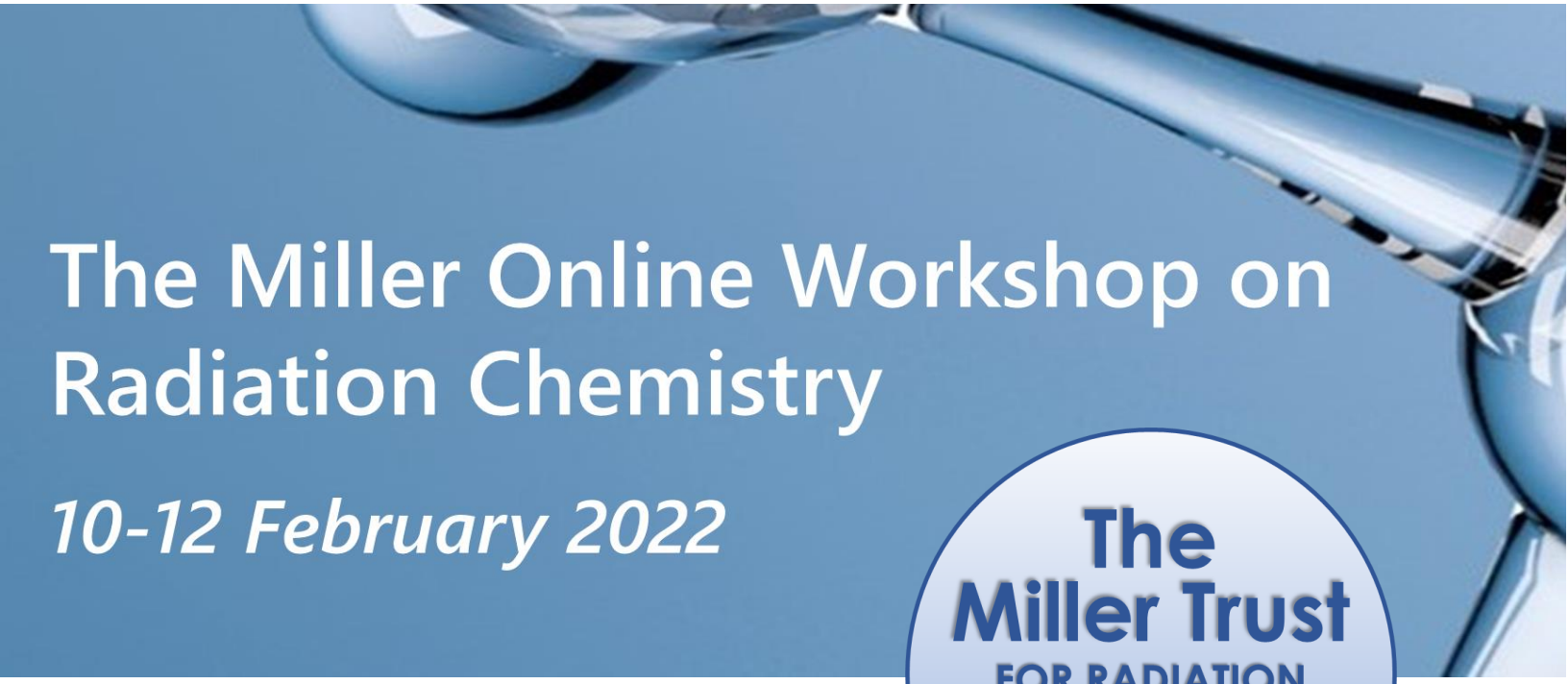
PROGRAMME AND BOOK OF ABSTRACTS



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The Miller Online Workshop on Radiation Chemistry

PROGRAMME AND BOOK OF ABSTRACTS

Edited by:
The Miller Trust Committee

February 2022

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WELCOME

Dear participants,

Science is, to a large extent, powered by meetings between peers. Meetings may lead to collaborations or to controversy, which in turn may initiate new ideas. The vital importance of meetings has become painfully clear during the last two years when we have had to cancel or postpone almost every conference, and visits to other labs have been very scarce. This affects early career scientists in particular, as the chances of building networks, being exposed to new ideas, and to present their own work have become very limited. When facing the inevitable decision of postponing the Miller Conference in 2021 to 2023, the Miller Trust Committee decided to host an online workshop on radiation chemistry. The main purpose of this initiative was to provide an opportunity for early career radiation chemists to present their work in front of the international community. During these three days, we will have the opportunity to listen to 36 presentations by early career scientists who are active in all the various fields of radiation chemistry. In addition to this, there will be five invited talks by senior radiation chemists and a poster session with 60 posters that will remain open for 24 h. As we are all aware, the more informal interactions with other people often turn out to be the more fruitful ones. Indeed, informal interactions are not really possible within the online format during sessions of oral presentations. However, the platform used for the poster session is very suitable for informal interactions. This is why we have decided to keep the platform open for 24 h.

We hope that you will all find the program interesting and enjoyable and that you will find chances to meet with new and old colleagues during the poster session. With more than 300 registered participants from 41 countries all over the world, there should be plenty of opportunities to expand your network.

We wish you all a productive and enjoyable meeting!

Mats Jonsson

Chair of the Miller Trust Committee

THE MILLER TRUST FOR RADIATION CHEMISTRY

The Miller Trust for Radiation Chemistry is an international society registered as a charity in the United Kingdom (registration # 802533) that was organised by former colleagues and friends of the late Dr. Nicholas Miller. The objects of the Trust are the advancement of public education concerning the chemical effects of radiation, in particular by holding conferences known as 'The Miller Conferences' in the UK and other countries in Europe, in the general subject area of radiation chemistry.

Miller Conferences have been held at two-year intervals since 1959 (with the exception of 2021 due to the COVID-19 pandemic), and have provided a European equivalent of the past Gordon Research Conferences on Radiation Chemistry, and now the International Conference on Ionizing Processes (ICIP).

All attendees of the most recent Miller Conference are members of the Miller Trust, which is managed by a committee of twelve members elected from the Trust.

The List of Miller Conferences

1st	1959	R. Roberts	Portmeirion, Wales
2nd	1961	F. S. Dainton	Portmeirion, Wales
3rd	1963	M. Magat	Rocamadour, France
4th	1965	W. Wild	Portmeirion, Wales
5th	1967	J. Kroh	Kazimierz: Poland
6th	1969	J. J. Weiss	Portmeirion, Wales
7th	1971	G. Semerano	Sardinia, Italy
8th	1973	J. H. Baxendale	Portmeirion, Wales
9th	1975	T. Gäumann	Bürgenstock, Switzerland
10th	1977	G. Scholes	Portmeirion, Wales
11th	1979	N. Th. Rakintzis	Nafplion, Greece
12th	1981	G. A. Salmon	Windermere, England
13th	1983	D. Schulte-Frohlinde	Hünfeld, Germany
14th	1985	A. J. Swallow	Windermere, England
15th	1987	R. Schiller	Sopron, Hungary
16th	1989	C. O. Phillips	Windermere, England
17th	1991	J. Belloni	Giens, France
18th	1993	P. Wardman	Windermere, England
19th	1995	Q. G. Mulazzani	Cervia, Italy
20th	1997	P. O'Neill, A. Johnson	Windermere, England
21st	1999	J. M. Warman	Doorwerth, The Netherlands
22nd	2001	N. Green	Windermere, England
23rd	2003	J. Mayer, J. L. Gebicki	Bialowieza, Poland
24th	2005	M. Spotheim-Maurizot, C. Houee-Levin	La Londe les Maures, France
25th	2007	S. M. Pimblott, N. Harridge	Buxton, England
26th	2009	E. Takács, L. Wojnárovits	Keszthely, Hungary
27th	2011	M. Jonsson	Tällberg, Sweden
28th	2013	I. Zilbermann, S. Goldstein	Dead Sea, Israel
29th	2015	N. Green	Windermere, England
30th	2017	C. Dispenza	Castellammare del Golfo, Sicily, Italy
31st	2019	F. Currell	West Cumbria, England
32nd	2023	S. Remita, S. Le Caër	Corsica, France (2021 conference postponed until 2023 due to COVID-19 pandemic)

ORGANISING AND SCIENTIFIC COMMITTEE

THE MILLER TRUST COMMITTEE (2017 – 2022):

Mohamad Al-Sheikhly (University of Maryland, USA)

Fred Currell (Dalton Cumbrian Facility, The University of Manchester, UK)

Clelia Dispenza (University of Palermo, Italy)

Vladimir Feldman (Lomonosov Moscow State University, Russia)

David Grills (Brookhaven National Laboratory, USA)

Mats Jonsson (KTH Royal Institute of Technology, Sweden) – CHAIR

Tanja Jurkin (Ruđer Bošković Institute, Croatia)

Sophie Le Caër (Université Paris Saclay, France) – VICE-CHAIR

Laura Leay (Science Writer, UK) – TREASURER

Samy Remita (Université Paris Saclay & Conservatoire National des Arts et Métiers, France) – SECRETARY

Piotr Ulański (Lodz University of Technology, Poland)

Israel Zilbermann (Ben-Gurion University of the Negev, Israel)

PROGRAMME TIMETABLE (CET Time Zone)

CET	Thu (10 Feb)	Fri (11 Feb)	Sat (12 Feb)
12:00	Opening of the Workshop	I3: X. Coqueret	I4: T. Sakurai
12:10	I1: B. G. Singh		
		O9: Y. M. Narode	O13: A. Rajpal
12:40	O1: S. Abou-Zeid	O10: M. O'Leary	O14: A. Ramos-Ballesteros
13:00	O2: J. Audouin	O11: D. Olsson	O15: A. Tegze
13:20	O3: A. Danvin	O12: S. B. Owusu	O16: E. C. Wu
13:40	O4: S. El Jamal	Coffee break	Coffee break
14:00	Coffee break	F9-F16: M. Lukianova, K. Omar, I. Sosulin, R. Sverdlov, J. Taibi, A. Volosatova, H. Weng, Y. Yang	I5: S. Ptasinska
14:10	I2: G. P. Horne		
			O17: H. Yu
14:40	O5: H. Hlushko	Poster Session (Gather platform)	O18: G. Zante
15:00	O6: K. Iwamatsu		O19: P. V. Zasimov
15:20	O7: C. Laube		O20: A. A. Zharikov
15:40	O8: I. Marić		Closing of the Workshop
16:00	Coffee break		
16:05	F1-F8: S. Bhattacharya, J. Conrad, V. D. Drabkin, B. Gu, R. Homlok, P. L. Huestis, S. Kabasa, J. Li		
16:45		Gather platform stays open 24 hrs until 14:30 (Feb 12)	

Legend: I – Invited Lecture (Senior Scientist)
O – Oral Presentation (Early Career Scientist)
F – Flash Presentation (Early Career Scientist)

PROGRAMME (CET Time Zone)

Thursday, 10 February	
12:00 – 12:10	**OPENING** OF THE WORKSHOP – **Mats Jonsson** (Sweden)
Chairperson: **Jai Pal Mittal** (India)	
INVITED LECTURE	
12:10 – 12:40	**I1: Prof. Beena G. Singh** (India) *Role of Gold Nanoparticles on the Free Radical Reaction of Antioxidants*
ORAL PRESENTATIONS (EARLY CAREER SCIENTISTS)	
12:40 – 13:00	**O1: Souad Abou-Zeid** (France) *Radiation Induced Reduction of Graphene Oxide: Application in Energy Storage*
13:00 – 13:20	**O2: Julien Audouin** (France) *Radiolytic Yields Along an Energetic Proton Track-End in Water Using an In-Line 2D Spectrophotometer*
13:20 – 13:40	**O3: Antoine Danvin** (France) *Dose-Rate Effects on the Yields of Hydroxyl Radical Under Irradiation by 1 MeV Electrons*
13:40 – 14:00	**O4: Sawsan El Jamal** (Sweden) *Radiation-Induced Dissolution of Uranium Carbide and Uranium Nitride in Aqueous Systems*
14:00 – 14:10	Coffee break
Chairperson: **Jay A. LaVerne** (USA)	
14:10 – 14:40	**I2: Dr. Gregory P. Horne** (USA) *The Role of Pulse Radiolysis in Advanced Nuclear Fuel Cycles*
ORAL PRESENTATIONS (EARLY CAREER SCIENTISTS)	
14:40 – 15:00	**O5: Hanna Hlushko** (USA) *Water Radiolysis on Surfaces of Various Zirconium Compounds*
15:00 – 15:20	**O6: Kazuhiro Iwamatsu** (USA) *Pulse Radiolysis Study of Metal Additives in Molten LiCl-KCl Salt*
15:20 – 15:40	**O7: Christian Laube** (Germany) *Probing Radiation Chemistry inside Electron Transmission Microscopy Liquid Cells*

15:40 – 16:00	**O8: Ivan Marić** (Croatia) *Synthesis of Magnetic Iron Oxide/Au Nanostructures Using the γ-Irradiation Method*
16:00 – 16:05	Coffee break
Chairperson: **James Wishart** (USA)	
FLASH PRESENTATIONS (EARLY CAREER SCIENTISTS)	
16:05 – 16:10	**F1: Susmita Bhattacharya** (USA) *Comparison of Transient Raman Spectra of Hydrated Dimer Radical Cations of Thiourea and Selenourea*
16:10 – 16:15	**F2: Jacy K. Conrad** (USA) *Multiscale Modeling of the Radical-Induced Chemistry of Acetohydroxamic Acid in Aqueous Solution*
16:15 – 16:20	**F3: Vladimir D. Drabkin** (Russia) *CH_3CN Complexes with Water and Carbon Dioxide and Their Radiation-Induced Transformations in Low-Temperature Matrices*
16:20 – 16:25	**F4: Bin Gu** (China) *Bragg's Additivity Rule and Core and Bond Model of Water Vapor Studied by Real-Time TDDFT Electronic Stopping Calculations*
16:25 – 16:30	**F5: Renáta Homlok** (Hungary) *Effect of Electron Beam Irradiation and the Presence of Antibiotics on the Population Dinamics of Resistant/Sensitive Bacterial Cultures in Model Wastewater Matrix*
16:30 – 16:35	**F6: Patricia L. Huestis** (USA) *Exploring Physical and Chemical Effects of Radiation on Explosives*
16:35 – 16:40	**F7: Stephen Kabasa** (Poland) *Computer Simulated Degradation of $CFCl_3$ Under Electron Beam*
16:40 – 16:45	**F8: Junyi Li** (Sweden) *Radiation Induced Dissolution of Studtite and Meta-Studtite*

Friday, 11 February	
Chairperson: **Chantal Houée-Levin** (France)	
INVITED LECTURE	
12:00 – 12:30	**I3: Prof. Xavier Coqueret** (France) *From Starch to Pullulan and Nanocellulose: The Radiation Chemistry of Polysaccharides Illustrated Through Examples*
ORAL PRESENTATIONS (EARLY CAREER SCIENTISTS)	

12:30 – 12:50	**O9: Yogitabali M. Narode** (India) *Catalytic Role of Gold Nanoparticles in Free Radical Induced Oxidation of Tyrosine*
12:50 – 13:10	**O10: Mel O'Leary** (UK) *Novel Radiation Driven Dynamics in Nanoparticle Sludges*
13:10 – 13:30	**O11: Daniel Olsson** (Sweden) *Effects of H_2O_2 Speciation in Radiation Induced Dissolution of UO_2-Based Nuclear Fuel*
13:30 – 13:50	**O12: Stephenson B. Owusu** (USA) *Pulse Radiolysis of Acetate, Malonate and Succinate in High Temperature Water*
13:50 – 14:00	Coffee break
Chairperson: **Krzysztof Bobrowski** (Poland)	
FLASH PRESENTATIONS (EARLY CAREER SCIENTISTS)	
14:00 – 14:05	**F9: Mariia A. Lukianova** (Russia) *Radiation-Induced Assembling of Benzene and Naphthalene Molecules from Molecular Aggregates and Complexes at Low Temperatures*
14:05 – 14:10	**F10: Karwan Omar** (France) *Effect of Biomolecule Environment on the Energy Deposition of Swift Charge Particles by First Principles Simulations*
14:10 – 14:15	**F11: Ilya S. Sosulin** (Russia) *Reactions of the Radiation-Induced Oxygen Atoms with Fluoroform and its Radiolysis Products: A Model Matrix Isolation and Ab Initio Study*
14:15 – 14:20	**F12: Roman L. Sverdlov** (Belarus) *The Influence of H/D Kinetic Isotope Effect and Structure of α-Diols on Their Radiation-Induced Fragmentation in Deaerated Aqueous Solutions*
14:20 – 14:25	**F13: Jamila Taibi** (France) *Radio-Grafting of Phosphorus Flame Retardant on Flax Fabrics: Pre-Irradiation Method*
14:25 – 14:30	**F14: Anastasia D. Volosatova** (Russia) *Radiation-Chemical Synthesis of C_2 and C_3 Nitriles in Cryogenic Media*
14:30 – 14:35	**F15: Hanqin Weng** (China & Japan) *γ-Radiation-Induced Hydroxylation on Boron Nitride Nanosheets for Selective Oxidative Dehydrogenation of Propane*
14:35 – 14:40	**F16: Yi Yang** (Sweden) *γ-Radiation Induced Synthesis of Ag Nanoparticles Using an Ionomer as Size Regulator*

14:40 – 16:40	**POSTER SESSION** (on Gather Platform)
16:40 – 14:30 (next day)	**Gather space will remain open for 24 hrs for scientific discussions and general socialising**

Saturday, 12 February	
Chairperson: **Erzsébet Takács** (Hungary)	
INVITED LECTURE	
12:00 – 12:30	**I4: Prof. Tsuneaki Sakurai** (Japan) *Fabrication of Organic Nanowires Developed by Radiation-Triggered Polymerization of Organic Molecules in Heavy Ion Tracks*
ORAL PRESENTATIONS (EARLY CAREER SCIENTIST)	
12:30 – 12:50	**O13: Aashini Rajpal** (France) *Detecting Superoxide Radical Anions in the Aqueous Medium, Resulting from Core-Shell Ionization Upon Exposure to Soft X-Rays*
12:50 – 13:10	**O14: Alejandro Ramos-Ballesteros** (USA) *Radiolytic Reduction of Li and Mg in Solid Chlorides*
13:10 – 13:30	**O15: Anna Tegze** (Hungary) *Radiation Induced Degradation of Fluoroquinolone Antibiotics in Aqueous Solution*
13:30 – 13:50	**O16: Eric C. Wu** (USA) *The Effects of Electrolytes on the Spectroscopy and Dynamics of Hydrated Electrons*
13:50 – 14:00	Coffee break
Chairperson: **Clara Wren** (Canada)	
14:00 – 14:30	**I5: Prof. Sylwia Ptasinska** (USA) *Importance of Radiation Chemistry to Low-Temperature Plasmas*
ORAL PRESENTATIONS (EARLY CAREER SCIENTISTS)	
14:30 – 14:50	**O17: Hao Yu** (Japan) *Radiation-Induced DNA Damage and Selective Protection by Antioxidants*
14:50 – 15:10	**O18: Guillaume Zante** (France) *Grafted Mesoporous Silicas for Radionuclide Uptake: Radiolytic Stability Under Electron Irradiation*

15:10 – 15:30	**O19: Pavel V. Zasimov** (Russia) *C_2H_2···CO complex and its Radiation-Induced Transformations: A Building Block for Cold Synthetic Astrochemistry*
15:30 – 15:50	**O20: Alexey A. Zharikov** (Russia) *One-Pot Radiation-Induced Preparation of Metal–Polymer Nanocomposites in Aqueous Solutions of 1-Vinyl-1, 2, 4-Triazole Containing Silver Ions*
15:50 – 16:00	**CLOSING** OF THE WORKSHOP – **Mats Jonsson** (Sweden)

POSTER SESSION (11 February, 14:40 – 16:40)	
P1	**Ahmed Alanazi** (CANADA), Abida Sultana, Jintana Meesungnoen, Jean-Paul Jay-Gerin *Early, Transient, Highly Acidic Spikes in the Radiolysis of Water at Very High Dose Rates: Relevance for FLASH Radiotherapy*
P2	**Atanu Barik** (INDIA) *Contrasting Reaction of Hydroxyl Radical with Respect to Ketone and Thioketone Group: A Case Study of Esculetin and Thioesculetin*
P3	**Malak Ben Salem** (TUNISIA), Amira Zaouak *Gamma Radiolysis of Sunset Yellow Dye in Aqueous Solutions*
P4	**Savannah Benjamin** (USA), Ginger Sigmon, Jay LaVerne, Peter Burns *Transformations of a Uranyl Hydroxide Phase: Probing Alteration Behavior through Humidity and Ionizing Radiation*
P5	Nicholas A. Till, Seokjoon Oh, David W. C. MacMillan, **Matthew J. Bird** (USA) *Pulse Radiolysis for Mechanistic Studies of Ni Metallaphotoredox Catalysis*
P6	**Yizhi Chen** (CHINA), Hanqin Weng, Geng Chen, Xinrui Zhang, Weiqun Shi, Mingzhang Lin *Study on Radiolysis Mechanism of Diamide Phenanthroline Extractant and Its Separation Performance for Actinides from Lanthanides*
P7	**Andrzej G. Chmielewski** (POLAND), Zbigniew Zimek, Yongxia Sun, Andrzej Pawelec, Marcin Sudlitz, Urszula Gryczka, Dagmara Chmielewska – Śmietanko, Sylwester Bułka *Radiation Chemistry and Technology for Environment Pollution Control*
P8	**Laboni Das** (INDIA), Soumyakanti Adhikari *Radiation Chemical Studies of Deep Eutectic Solvents and Application as Host Matrix in Radiation-Assisted Synthesis of Photoluminescent Tin Oxide Nanospheres*
P9	**Aki Goto** (JAPAN), Takashi Tanji, Masahito Tagawa, Koji Michishio, Toshitaka Oka, Shinichi Yamashita *Atomic-Oxygen-Induced Microstructure Formation on Polymers: Higher-Order Structure Effects on Morphologies*
P10	**Apurav Guleria** (INDIA) *Radiation-Assisted Synthesis of Photoluminescent Cyclodextrin Passivated Tellurium Nanocomposites: Mechanistic Studies and Biomedical Applications*
P11	**Zifang Guo** (CHINA), Yu Yang, Limin Jiao, Geng Chen, Yunliang Lin, Jia Tang, Mingzhang Lin *The Study on the γ-Radiolysis of Ammonia Solution*
P12	**Alaa Huwaidi** (CANADA), Bhavini Kumari, Gabriel Robert, Brigitte Guérin, Léon Sanche, J. Richard Wagner *Profiling DNA Damage Induced by the Irradiation of DNA with Gold Nanoparticles*

P13	**Marwa Jabberi** (TUNISIA), Afef Najjari, Habib Chouchane, Hadda Imene Ouzari-Cherif, Ameur Cherif, Ahmed Landoulsi, Haïtham Sghaier *Preliminary Study of Natural Radionuclides and Radiological Risk Assessment of a Forest Soil in Tunisia*
P14	Susmita Batharachaya, **Ireneusz Janik** (USA) *An Attempt to Correlate Charge Distribution in Hydrated Assymetric Hemi-Bonded Radical Anions with Their Structural Properties*
P15	**Limin Jiao** (CHINA), Yi Wang, Zhihao Wu, Mingzhang Lin *Effect of Gamma and Neutron Irradiation on Properties of Boron Nitride/Epoxy Resin Composites*
P16	**Olga V. Karmanova** (RUSSIA), Sergey G. Tikhomirov, Anatoly A. Khvostov, Zhanna S. Shashok, Sergey N. Kayushnikov *Development of Approaches to the Regeneration of Rubber Products Using Irradiation*
P17	**Meysam Khosravifarsani** (CANADA), Samia Ait-mohand, Benoit Paquette, Léon Sanche, Brigitte Guérin *Development of Low Energy Electron Sources as Novel Chemo-Radio Therapeutic (CRT) Agents: In-vitro Study of ^{64}Cu/NOTA-Terpyridine Platinum in Colorectal Cancer Cell*
P18	**Janina Kopyra** (POLAND), Paulina Wierzbicka, Adrian Tulwin, Guillaume Thiam, Ilko Bald, Franck Rabilloud, Hassan Abdoul-Carime *Low-Energy Electron Attachment to Metabolites: Oxaloacetic and Citric Acids*
P19	**K. Kovács** (HUNGARY), Á. Simon, T. Tóth, L. Wojnárovits *Free Radical Reactions of Atenolol and Propranolol by Pulse Radiolysis*
P20	**Bhavini Kumari** (CANADA), Alaa Huwaidi, Gabriel Robert, Pierre Cloutier, Andrew Bass, Léon Sanche, J. Richard Wagner *Shape Resonances in DNA: Very Low Energy Electron (VLEE) Induced DNA Damage*
P21	**Ilyes Mahti** (FRANCE), Dominique Guillaumont, Laurence Berthon *Effect of Metal Complexation on the DOTA Radiolysis*
P22	**Takuya Majima** (JAPAN), S. Mizutani, K. Kitajima, Y. Mizunami, H. Tsuchida, M. Saito *Mass Spectrometric Study of MeV-Ion-Induced Reactions on Submicron Ethanol Droplet Surfaces*
P23	**Camille Méhault** (FRANCE), S. Saintignon, C. Le Pennec, S. Faure *Modelling the Gas Generation of Actinide Bearing Materials in Storage Containers*
P24	**Daniel Muñoz-Santiburcio** (SPAIN), Bin Gu, Fabiana Da Pieve, Fabrizio Cleri, Emilio Artacho, Jorge Kohanoff *Solvation Effects on Proton Irradiation of DNA*

P25	**Maddalena Negrin** (ITALY), E. Macerata, F. Concia, E. Mossini, G. Magugliani, S. Sancassani, M. Mariani *How to Use a MOOC in Radiation Chemistry: A Toolkit for Teachers*
P26	**Vagisha Nidhi** (FRANCE), Fabienne Testard, Florent Malloggi, Jean-Philippe Renault *Radiotactic Colloids: Towards Decontamination Nanorobots*
P27	**Nikolina R. Nikolić** (SERBIA), Aleksandra N. Radosavljević, Jelena P. Spasojević, Una M. Stamenović, Vesna V. Vodnik, Zorica M. Kačarević-Popović *Au-PNiPAAm Hydrogel Nanocomposites as Photoactuators for Direct Optical to Mechanical Energy Conversion*
P28	**Ena Pezić** (CROATIA), Helena Mijić, Nives Matijaković, Branka Mihaljević, Katarina Marušić *Application Methods and Irradiation Atmosphere for Radiation Crosslinked Polymer Nanocoatings*
P29	**Phan Viet Cuong** (VIETNAM), Nguyen Ngoc Duy, Le Xuan Vinh *Preparation of Oligochitosan by Gamma Irradiation of Solution Chitosan with Hydrogen Peroxide and Survey of Antioxidant Activity*
P30	**Dmitry E. Polyansky** (USA), David C. Grills, Mehmed Z. Ertem, Ken T. Ngo, Etsuko Fujita *Pulse Radiolysis Reveals the Role of Bimetallic Interactions in Enhancement of Catalytic CO_2 Reduction by a Macrocyclic Cobalt Catalyst*
P31	**Martin Precek** (CZECH REPUBLIC), Petr Kubelik, Ludek Vysin, Uli Schmidhammer, Jean-Philippe Larbre, Alexandre Demarque, Pierre Jeunesse, Mehran Mostafavi, Libor Juha *Fluorescence Chemical Dosimetry of Ultrashort Electron Pulses*
P32	**Ella Schaefer** (UK), B. Villagomez Bernabe, M. O'Leary, M. Bankhead, F. Currell *A Monte Carlo Study of Nanoparticles Relevant to Nuclear Waste and Healthcare*
P33	Ákos Horváth, Norbert Nagy, Gábor Vértesy, **Robert Schiller** (HUNGARY) *Effect of Ion Irradiation on the Work Function of Metals*
P34	**Pavlina I. Schmitz** (UK, GERMANY) *Funding Opportunities for Mobility and Radiation Chemistry Research in the EU Horizon Europe*
P35	**Ekaterina S. Shiryaeva** (RUSSIA), Irina A. Baranova, Elizaveta V. Sanochkina, Svetlana V. Kameneva, Glafira S. Taran, Alexander V. Belousov, Vladimir I. Feldman *Concerning the Mechanism of Radiation Sensitization by Metal Oxide Nanoparticles under X-ray Irradiation of Oxygen-Free Aqueous Organic Solutions: A Spin Trapping Study*

P36	**Abida Sultana** (CANADA), Jintana Meesungnoen, Jean-Paul Jay-Gerin *On the Radiolytic Oxygen Depletion in the Ultra-High (FLASH) Dose-Rate Radiolysis of Water in a Cell-Like Environment: Influence of e^-_{aq} and $^{\bullet}OH$ Competing Scavengers*
P37	**Ivana Tartaro Bujak (**CROATIA), K. Blažek *Radiation Induced Degradation of Doxazosin*
P38	**Svenja Trapp** (THE NETHERLANDS), Robin de Kruijff, Elisabeth Paulßen *Microfluidic Solvent Extraction of Cyclotron Produced ^{68}Ga from Zinc Nitrate Solutions. Towards an Automated Production Loop*
P39	**Irina S. Tretyakova** (RUSSIA), Vsevolod I. Borovkov *Solvent-Related Radical Ions in Irradiated Diethyl Carbonate*
P40	**Rodion A. Vinogradov** (RUSSIA), Alexey A. Zharikov, Elena A. Zezina, Alexander S. Pozdnyakov, Vladimir I. Feldman, Alexandr L. Vasiliev, Alexey A. Zezin *The Radiation-Induced Preparation of Ultrasmall Gold Nanoparticles in Au(III) Complexes with Units of Poly(1-Vinyl-1,2,4-Triazole) and Poly(1-Vinyl-1,2,4-Triazole) – Poly(Acrylic Acid)*
P41	**Mariya Vyushkova** (USA), Brian Rost, Barbara Jones, Aaila Ali, Charlotte Cullip, Alexander Vyushkov, Jarek Nabrzyski *Quantum Computing for Radiation Chemistry: Simulation of Magnetic Field Effects on Pulse Radiolysis on IBM Q*
P42	**Runze Wang** (THE NETHERLANDS), Hubert Wolterbeek, Antonia Denkova *Core-Shell Structured Gold Nanoparticles as Carrier for ^{166}Dy/^{166}Ho in Vivo Generator*
P43	**Peng Zhang** (CHINA), Hanqin Weng, Mingzhang Lin *Preparation of Reduced Graphene Oxide Composite Aerogel by Radiation Method and Its Adsorption Performance of Organic Pollutants*
P44	**Yi Zheng** (CANADA, CHINA), Xuran Wang, Yanfang Dong, Léon Sanche *Transient Anions in Chemoradiation Therapy: Enhancement of Detrimental Clustered Lesions and Crosslinks Induced by 1-20 eV Electrons to Cisplatin-DNA Complexes*
F1 – F16	**All the flash presentations have an associated poster.**

INVITED LECTURES

Role of gold nanoparticles on the free radical reaction of antioxidants

Beena G. Singh[1,2]

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Nanoparticles derived from noble metals are extensively studied for their catalytic properties. Recently, few reports have indicated that the stability of free radicals generated by ionizing radiation is affected in the presence of gold nanoparticles (GNP). This property is important to understand the fundamental process involved in radio-sensitization by GNP. Antioxidants which protect the cells from free radicals can act as radio-modifiers in presence of GNP. We have initiated research in understanding the fate of the free radical in presence of GNP, and a few examples from our recent studies are discussed below [1-3].

Two structural isomeric selenium compounds, linear, bis(ethan-2-ol)selenide (SeEOH), and cyclic, DL-trans-3,4-dihydroxy-1-selenolane (DHS), were compared for their antioxidant activity. It was found that DHS exhibited antioxidant activity while SeEOH showed pro-oxidant activity. The pro-oxidant activity in SeEOH aroused due to the formation of reducing radical and formaldehyde on reacting with free radicals like hydroxyl ($^{\bullet}$OH) radical. Similar study with SeEOH in the presence of GNP did not show formation of formaldehyde. The differential activity in presence of GNP was attributed to the increase in stability of the intermediate transient in presence of GNP [2].

In another study, oxidative reaction of tyrosine with $^{\bullet}$OH radical in presence of GNP was investigated. In absence of GNP, Try reacted with $^{\bullet}$OH radical to form dityrosine (DT) as minor product. However, in presence of GNP the yield of DT increased significantly. Mechanistic investigation indicated stabilization of tyrosyl, the precursor of DT dominated in the presence of GNP [3].

The above results indicated that GNP may act as a Lewis acid which enhanced the radical cation formation and thereby promotes dimerization of the radicals. Also, the nature of the product formed may dictate the biological outcome of the radiation induced chemical reaction.

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Abstract of poster/oral presentation (online) for The Miller Online Workshop on Radiation Chemistry, 10-12 February 2022, organized by the Miller Trust for Radiation Chemistry, UK

(Dr. A. K. Tyagi)
Director, Chemistry Group

The Role of Pulse Radiolysis in Advanced Nuclear Fuel Cycles

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The effects of ionizing radiation are ubiquitous throughout all aspects of a nuclear fuel cycle. The complexity and intensity of these effects are greatest during reactor operations and in the management of used nuclear fuel and waste [1,2]. Radiation-induced processes typically promote the chemical transformation of molecules and materials with the formation of potentially detrimental degradation products and corresponding changes in physical and chemical properties, which ultimately impact the effectiveness and longevity of nuclear technologies. Consequently, a molecular-level understanding of radiation effects over multiple *time*, *distance*, and *material domains* is essential for the innovation and deployment of next generation nuclear technologies. Attaining this knowledge necessitates a firm grasp of radiation-induced reaction kinetics, for which pulsed electron radiolysis is the methodology of choice [2]. Presented here are several recent studies from our group that demonstrate the critical role of pulsed electron radiolysis techniques in the advancement of our understanding of radiation-induced chemistry under advanced nuclear fuel cycle conditions.

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From Starch to Pullulan and Nanocellulose: The Radiation Chemistry of Polysaccharides Illustrated Through Examples

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The behavior of polysaccharides submitted to ionizing radiation is roughly described by their general trend towards chain scission which primarily depends on the structure of the polymer, its pre-irradiation chemical treatment, and the degree of hydration. Though certain applications aim at decreasing the polysaccharides molecular weight by radiation-induced chain scission, for biomass deconstruction, or to produce various types of oligomers, the degradative behavior is often a limitation in developing new applications based on radiation-induced modification such as grafting. [1,2]

To overcome the radiation-induced degradation of polysaccharides, processing methods with corrective actions involve either blending them with monomers that polymerize and form crosslinks under ionizing radiation or converting reactive side-groups with appropriate functionalities, trying to balance chain scission by simultaneous cross-linking. The first approach was applied to thermoplastic starch blends, as promising bio-based substitutes to plastics, to mitigate the water sensitivity and to reduce retrogradation of amorphized starch by blending it with lignin or with allyl urea followed by electron beam (EB) processing. EB-irradiation improves the initial bulk and surface properties of the obtained materials and to limit the changes in structural features and mechanical performances with time. The reactivity of the blends submitted to radiation was studied in terms of kinetics and chemical mechanism to provide sufficient control over the transformations occurring at the molecular and macromolecular levels. [3-6]

Basic studies with maltodextrin and pullulan as model compounds mixed with low MW aromatic additives such as cinnamyl alcohol (CA) revealed a strong dependence of the radiation-induced degree of modification on the (i) chemical composition of the blend, and (ii) inter-molecular associations between the blends constituents. [7,8] The protective effect against radiation provided by the aromatic additives is emphasized and quantified by determining the changes in radiation chemical yields for scission *G(S)* and for cross-linking *G(X)* for hydro-alcoholic pullulan blends containing various amounts of cinnamyl alcohol. [9-11] Activities involving the treatment under radiation of other polysaccharides under various physical forms provide additional information giving a composite picture of this specific domain of radiation chemistry.

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Fabrication of Organic Nanowires Developed by Radiation-Triggered Polymerization of Organic Molecules in Heavy Ion Tracks

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In this talk, the author reports a unique method to develop organic nanowires with a controlled length, radius, and number density, via particle beam radiation-triggered polymerization of organic films.[1] High-energy particle irradiation of organic films from the vertical direction resulted in polymerization/cross-linking reactions of the small organic molecules within the cylindrical ion tracks to give polymerized nanowires (Figure 1). After the nanowires formed by irradiations, the use of a wet process (development) or dry process (sublimation) determines the orientation of the nanowires. The former allows the knocked-down nanowires while the latter gives vertically-aligned standing nanowires. The author will introduce the recent examples of functional nanowire bundles from porphyrin molecules[2] and standing nanowires from various halogenated/unsaturated aromatic molecules with structure-directed water repellency (Figure 2).[3]

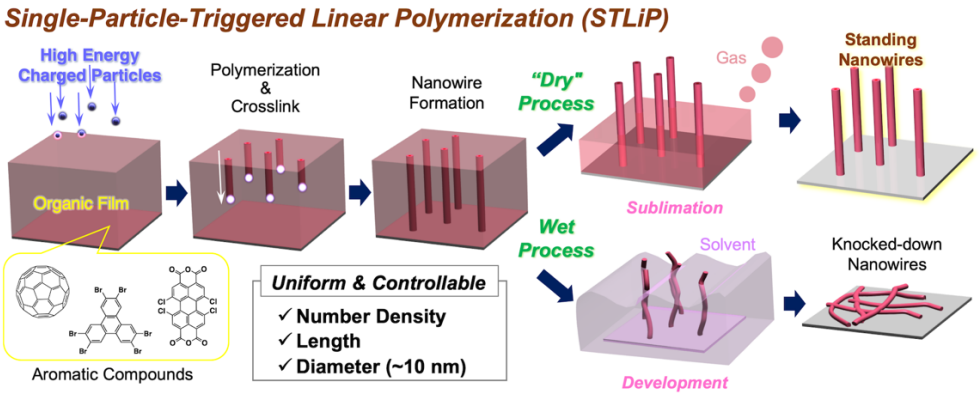

Figure 1. Schematic illustration of nanowire fabrication processes via heavy ion irradiation.

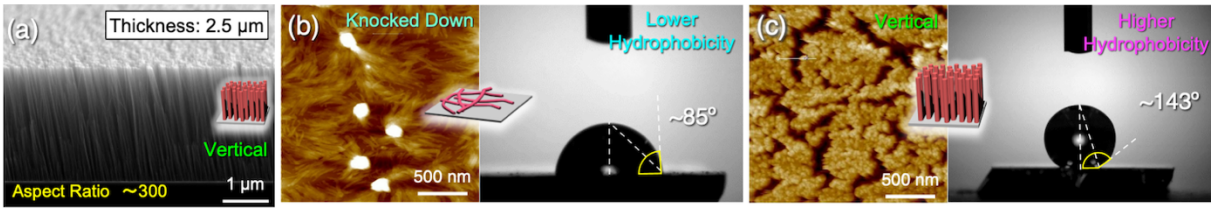

Figure 2. (a) Typical SEM images of standing nanowires based on C_{60}. AFM images and water contact angle snapshots of (b) knocked-down and (c) standing nanowires based on C_{60}.

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Importance of Radiation Chemistry to Low-Temperature Plasmas

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Recent advances in plasma technology have achieved a novel radiation type formed due to electric discharges under ambient conditions, called low-temperature plasmas (LTPs), which open up a wide range of potential applications in the industrial and medical areas. However, despite the rapid growth in interest in this non-traditional source of radiation, there is still a lack of fundamental and comprehensive knowledge of chemistry that plasma irradiation induces in multiphase systems. A thorough understanding is of particular importance for clinical applications, and although some preliminary clinical trials have been reported, many challenges remain that need to be addressed and tackled [1].

We recently developed and have employed several different techniques to characterize both the physical and chemical properties of LTPs and their effect on DNA and cancer cells [2,3]. The survey of these studies conducted in our laboratory will be presented at the workshop.

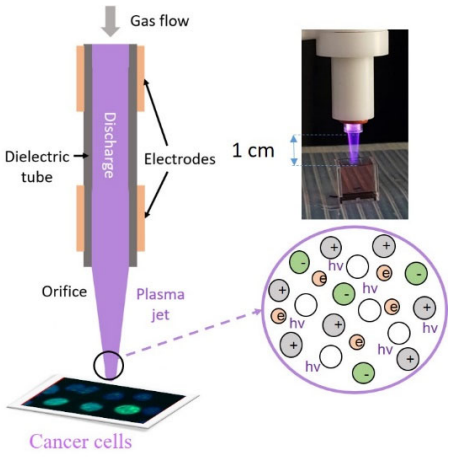

Figure 1. Schematic view and photograph of the low-temperature plasma (LTP) source used to irradiate biological samples. LTP consists of chemical components that are biologically reactive species such as free electrons and radicals, atoms, and molecules either in neutral or charged form, and physical components such as electromagnetic fields, photons, shock waves, and heat.

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EARLY CAREER SCIENTIST ORAL PRESENTATIONS

Radiation induced reduction of graphene oxide: application in energy storage

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Due to their exceptional properties, graphene and its composites are considered as revolutionary materials in the fields of energy, electronics, sensors and health. However, manufacturing such materials remains difficult and expensive while used techniques often yield to low quality materials and generate toxic organic products, which hampers their industrialization.

In this context, starting from commercial graphene oxide (GO), we recently developed a new original radiolytic route (***Figure 1***) to produce highly reduced graphene oxide (rGO). The yield of reduction was determined by a dose effect study, while the physicochemical properties of the as-prepared materials were evaluated by the way of complementary techniques, such as UV-Visible, ATR -FTIR, EDX and Raman spectroscopies, as well as SEM and TEM microscopies. Besides, thermal stability of rGO, as determined by thermogravimetry, and capacitive properties of these materials in the field of energy storage, as highlighted by electrochemistry, appear as very encouraging results.

Our methodology was finally extended to the one-pot preparation of hybrid nanocomposites, made of rGO on the one hand and either metal nanoparticles or conducting polymers on the other hand, giving a glimpse of future industrial applications.

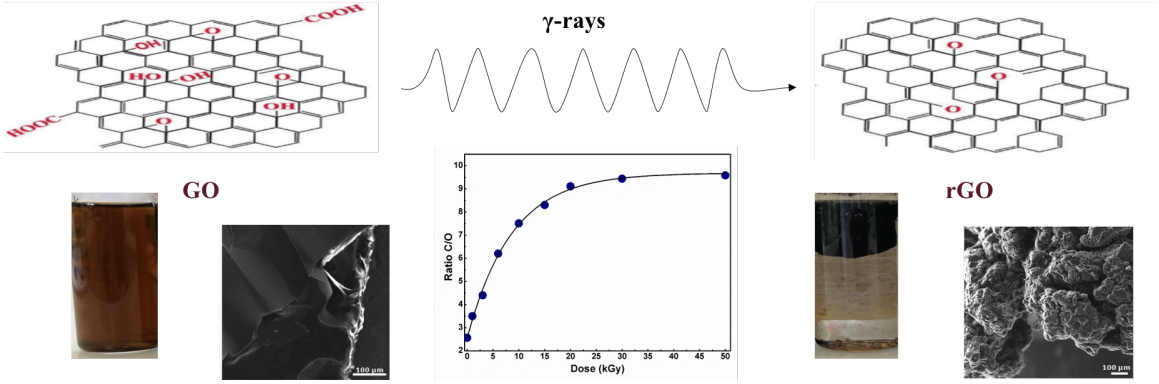

Figure 1. Preparation of rGO by radiation induced reduction of GO

Radiolytic Yields along an Energetic Proton Track-End in Water using an in-line 2D Spectrophotometer

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The track end of proton in water is indeed characterized by a sharp and intense Bragg peak, which is used in hadrontherapy to maximize the dose in the tumor cells. Radiolytic yields have been determined for MeV-protons to better understand the physical-chemical processes occurring in proton tracks. The yield values were either average yields, including Bragg peak[1], or differential yields, measured on portions of track with narrow energy distribution[3] using various energies of beams. As far as we know, no direct determinations of radiolytic yields along the last 1cm of a proton beam have been conducted. This kind of results would help to refine and adjust the models used in computational codes widely used in radiotherapy. We propose to carry out Fricke dosimetry and e^-_{aq} and $^\bullet OH$ yield determination through the implementation of an original absorbance/fluorescence setup in line with proton beams of 25, 30 and 65 MeV provided by cyclotrons (CEMHTI @ Orléans and CAL @ Nice). The originality of this setup is the use of a 20-fibers bundle, which conveys transmitted or fluorescence light from 20 positions in the sample, to a monochromator and a CCD camera. Recordings of sequences are performed in a few 10s of seconds under proton radiation.

We combined a scavenging method and fluorescence to determine the yield values by using solutions of Rezasurin (resp. Amplex Red) that reacts with e^-_{aq} (resp. with $^\bullet OH$) to produce resorufin (RN) that is stable and extremely fluorescent under excitation light at 510 nm. We propose to present the first results along the track of dosimetry and yields in order to discuss them by comparison with the literature.

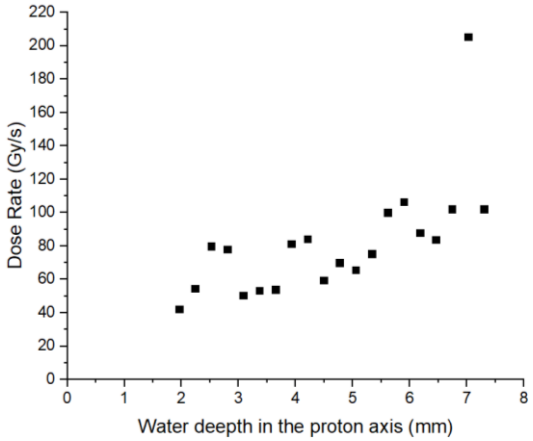

Figure 1. Dose rate along the track of 30 MeV proton beam (CEMHTI cyclotron) of 0.5 nA in Fricke's solution. Each point corresponds to one fiber in the 20-fiber bundle.

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Dose-rate effects on the yields of hydroxyl radical under irradiation by 1 MeV electrons

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Particle therapy or "hadrontherapy" is a method of cancer treatment, which uses ion beams instead of X-rays as in classical radiotherapy. This technique is distinguished by the ions Bragg peak, which allows better targeting of the tumors and better preservation of the healthy tissues. FLASH radiotherapy is a modality that gives high hopes, as it has a lower impact on healthy tissue compared to conventional therapy [1]. Its principle is based on irradiation with very high dose rates (> 40 Gy/s) in a very short time. At very high dose rates, the reactive species formed in the track of an ionizing radiation can react with that formed in another track, which will have an impact on their yields. FLASH effects has been mostly studied with electron beams.

In our lab, we are developing a systematic study of the chemical effects of the species produced by water radiolysis on protein biomolecules. For this purpose, we are studying water radiolysis by measuring radiolytic yields of its species ($HO^{\bullet}$, e^-_{aq}, H_2O_2…) as well as radiolysis of amino acids, peptides and proteins. Most of our irradiations are performed with ions, but other ionizing radiations (X-rays, γ, electrons) are used to highlight ions specificities [2].

This presentation will focus on the measurements of the yields (G) of the hydroxyl radical ($HO^{\bullet}$) with dose rates from 0.1 to 2000 Gy/s, under irradiation by 1MeV electrons (Van De Graaff accelerator, Aerial-CRT). These measurements were performed with two different molecular scavenging probes (C3CA and KBr/formate), and the kinetics of the radical were reconstructed from 370 ps to 1480 ns. A significant dose rate impact has been observed (*Figure 1*), with different thresholds depending on the scavenging time.

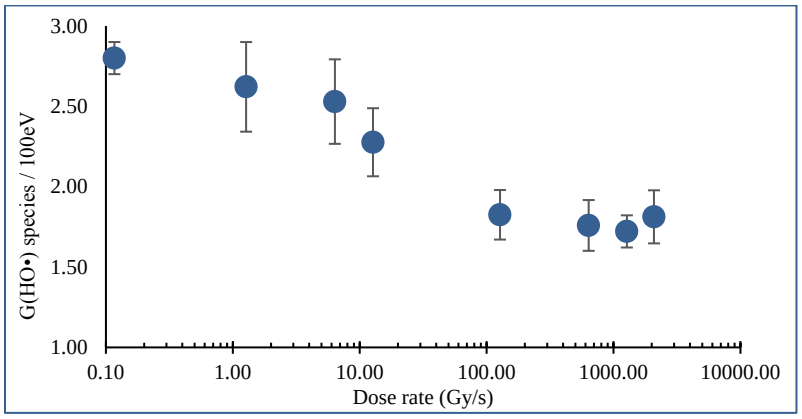

Figure 1. Evolution of G($HO^{\bullet}$) depending on the dose rate for a scavenging time of 74ns.

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Radiation-Induced Dissolution of Uranium Carbide and Uranium Nitride in Aqueous Systems

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Alternative materials to UO_2 are investigated as potential fuels for Generation IV nuclear reactors. Uranium carbide (UC) and uranium nitride (UN) are considered as potential substitutes for UO_2 for their better thermal conductivity and higher fissile material density.[1,2] Since these new materials will become part of the nuclear fuel cycle, they will at some point be treated as spent nuclear fuel and could end up being stored in deep geological repositories for long periods of time. As part of a safety assessment, it is essential to understand the behavior of UC and UN in contact with water. Spent nuclear fuel materials may display reactivity directly towards groundwater and the ionizing radiation emitted from the fuel will create even more reactive conditions due to water radiolysis.

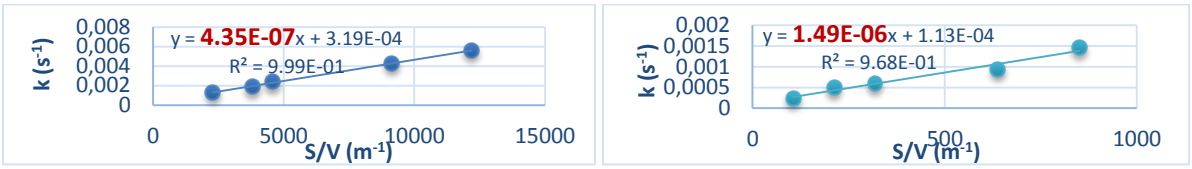

Figure 1. First-order rate constant k (s^{-1}) as a function of solid surface area over total solution volume ratio [S/V (m^{-1})] for different amounts of UC (left) and UN (right) in 25 mL 10 mM $NaHCO_3$ solution after exposure to 0.2 mM H_2O_2.

As a result, different oxidants are produced among which H_2O_2 has been shown to be the most important.[3] The oxidants oxidize solid uranium compounds to soluble U(VI) and thereby drive the dissolution process. To compare the reactivity of the new fuel materials, UC and UN were exposed to H_2O_2 in aqueous solutions with and without HCO_3^-. The oxidative dissolution was studied using different amounts of UC and UN (different solid surface area to fixed total solution volume) after adding 0.2 mM of H_2O_2 into the aqueous systems. The results in Figure 1 representing the second order rate constants indicate that UN is 3 times more reactive towards H_2O_2 than UC[4] and UO_2[5] is even less reactive. The dissolution yield (amount of dissolved uranium per consumed H_2O_2) was lower for UN than for UC which in turn has a lower dissolution yield than UO_2. UC and UN powders in aqueous suspensions were also exposed to gamma radiation. The results of these experiments will be discussed in view of the relative impact of the radiolytic oxidants.

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Water Radiolysis on Surfaces of Various Zirconium Compounds

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Ionizing radiation causes water radiolysis, producing free electrons, radicals, and their recombination products, including oxygen, hydrogen, and hydrogen peroxide. The yields of various radiolysis products may change, depending on many factors, including the presence of soluble species and solid surfaces. It was shown that water adsorbed on surfaces of various oxides, including zirconium oxide [1], undergoes radiolysis under ionizing radiation, producing a large amount of hydrogen. The presence of hydroxyl groups on the zirconium oxide surface facilitates adsorption of water molecules and increases hydrogen production under irradiation [2]. This work further explores zirconium materials, comparing zirconium oxide with nitride and carbide. Slurries containing 20-90 % of water demonstrated similar hydrogen yields for different zirconium compounds when irradiated with 100 kGy of gamma radiation, suggesting that hydrogen production is led by bulk and surface water. In contrast, hydrogen production by solid powders, containing only adsorbed water, was significantly higher for zirconium oxide, than for nitride, while no detectable hydrogen was produced by carbide. These results correlate with very low amount of adsorbed water and surface hydroxyls on zirconium carbide and nitride, suggesting important role of hydroxyl groups and chemisorbed water in water radiolysis on the surface.

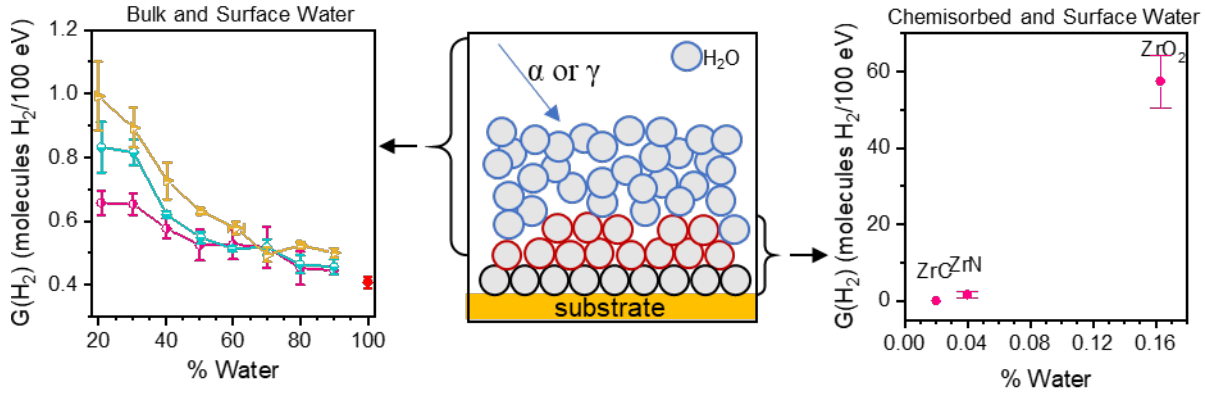

Figure 1. Schematics describing presence of water layers at the solid surfaces (middle). Bulk and surface water more likely affect water radiolysis in slurries (left), while chemisorbed and surface water are responsible for hydrogen production by solid powders with adsorbed water (right).

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Pulse Radiolysis Study of Metal Additives in Molten LiCl-KCl Salt

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The molten salt reactor concept, where nuclear fuel is dissolved in a molten salt media that also serves as the heat transfer fluid, is a leading candidate for next generation nuclear reactors. There are many scientific questions unsolved such as salt property, interaction with materials and so on. Radiation induced species are known to change their kinetics in the media and minor additive affect them. Recent paper shows radiation protection effect by chromium containing material and its reaction kinetics need to be clarified[1]. This necessitates understanding of radiation effects on molten salt media and reactor materials to support the design and development of such reactors. Several pioneering pulse radiolysis molten salt experiments observed transient species and their kinetic[2,3], however, there are numerous fundamental questions need to be answered. These include determination of the initial yields and reactivity of the primary radiolytic species from molten salt radiolysis, i.e., the solvated electron (e_s^-), chlorine atom ($Cl^\bullet$), and dichloride radical anion ($Cl_2^{\bullet-}$). Here we report on the reaction kinetics for the e_{ss}^- and $Cl_2^{\bullet-}$ in molten LiCl-KCl eutectic salt doped with metal ions at 400-600 °C. Experiments were performed using the Brookhaven National Laboratory Laser-Electron Accelerator Facility (LEAF)[4] using a recently-developed high-temperature sample holder.[5]

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Probing Radiation Chemistry inside Electron Transmission Microscopy Liquid Cells

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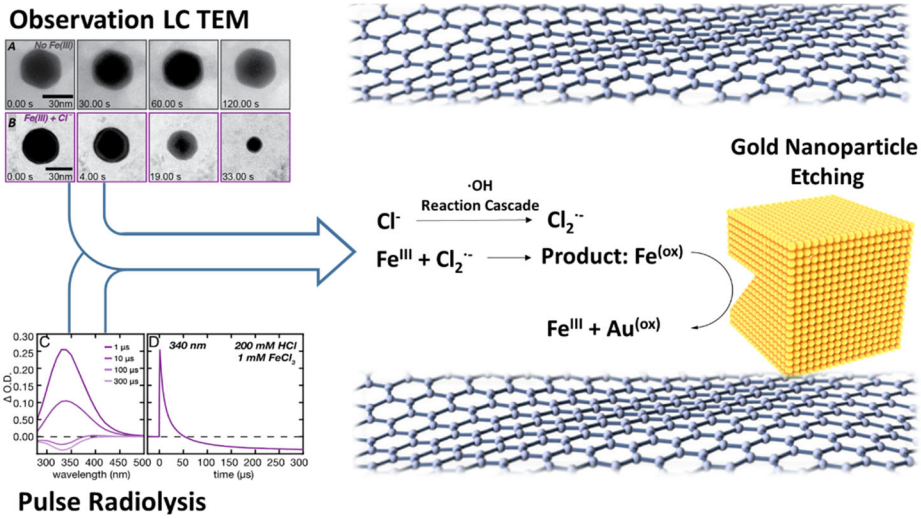

Graphical Abstract: *Liquid cell TEM and Pulse Radiolysis investigations probing the mechanism of gold nanoparticle etching in Liquid cell TEM experiments.*

Transmission electron microscopy (TEM) is a powerful tool to investigate mechanisms and structures at the nano and atomic size range. Using graphene liquid cells (LC), the observation of Transmission nanoparticle growth and etching in suspension is possible. During the last years these experiments provided valuable input for the understanding of nanoparticle formation and stability. Herein, one key factor for the understanding and interpretation of the LC-TEM results is the understanding of the occurring radiation chemical processes inside the liquid cell. To probe these processes time resolved-pulse radiolysis is a powerful tool. Nevertheless, the complementarity of LC-TEM and pulse radiolysis investigation need to be proven. To demonstrate the complementarity, the acidic etching of gold nanoparticles in presence of iron (III) ions was investigated. This study combines the visual observation of the etching kinetics during the LC TEM experiments with time resolved transient monitoring of possible reactants involved during the etching. Our results provide a new understanding of the involved radiation chemical processes during the etching process indicating iron intermediates as possible reactants.

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Crook MF, Laube C, Moreno-Hernandez IA, Kahnt A, Zahn S, Ondry JC, Liu A, Alivisatos AP., *J Am Chem Soc*. **2021**;143(30):11703-11713.

Synthesis of magnetic iron oxide/Au nanostructures using the γ-irradiation method

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Superparamagnetic iron oxide nanoparticles (MNPs) due to their unique magnetic and electrical properties have applications as biosensors, contrast agents, in drug delivery and for hyperthermia cancer treatments. For these uses, the surface of the particles should be modified with a suitable coating. Gold is one of the favored coatings because it is non-toxic, biocompatible, chemically inert, can protect MNPs from oxidation without significantly reducing magnetic properties and enables surface functionalization. It also has special optical properties. Such composite nanostructures have promising applications and advantageous properties compared to individual Au and MNPs. In this work we have used γ-irradiation as an efficient and ecologically friendly technique for the synthesis of magnetic nanoparticles. γ-irradiation has an advantage of inducing electrons and other reducing species homogeneously throughout the sample. The iron(III) chloride alkaline aqueous solutions were purged with nitrogen and γ-irradiated with addition of 2-propanol. DEAE-dextran was used as growth and stabilizing agent of MNPs in suspensions. The phase composition, stoichiometry, and morphology of MNPs were controlled by adjusting γ-irradiation dose. Irradiation with doses 10-36 kGy resulted in the formation of 4 nm spherical substoichiometric magnetite NPs, whereas at higher dose (50 kGy or more) the major phase was magnetic δ-FeOOH (feroxyhyte) in the form of nanodiscs. The reduction of Fe^{3+} to ferrous Fe^{2+} ions was quantitatively determined using the 1,10-phenanthroline spectrophotometric method. The reduction proceeds fast in the beginning stages of irradiation (up to 30 kGy, ~65% Fe^{3+} reduced), slows down, and reaches 100% reduction at ~75 kGy. The reducing power of Fe^{2+} in irradiated suspensions was explored to synthesize composite iron oxide/Au nanostructures by the addition of aqueous solutions of $HAuCl_4$ into the irradiated suspensions. Microstructural and morphological analysis showed that the simultaneous oxidation of $Fe(OH)_2$ and reduction of Au^{3+} resulted in the formation of composite δ-FeOOH nanodiscs decorated with spherical Au nanoparticles. The density and size of Au NPs depended on the amount of added $HAuCl_4$ aqueous solution.

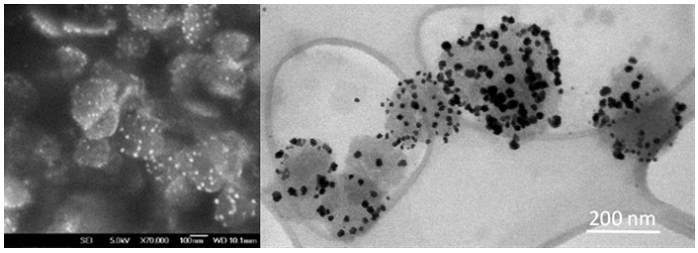

Figure 1. SEM and HRTEM micrographs of thin δ-FeOOH nanodiscs decorated with Au NPs.

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Catalytic role of gold nanoparticles in free radical induced oxidation of tyrosine.

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Amino acids are building block of proteins, linked through a peptide bond. Tryptophan, tyrosine, phenylalanine are the important aromatic amino acids. Among these only tryptophan and tyrosine exhibit fluorescence. Tyrosine plays a vital role in protein synthesis and neurotransmitter production.

We synthesized gold nanoparticles by using Creighton's chemical reduction method[1]. The free radical induced oxidation in tyrosine and the role of gold nanoparticle in the oxidation mechanism was investigated using UV–visible spectroscopy, fluorescence, high resolution mass spectroscopy, steady state radiolysis and pulse radiolysis.

The mechanism of free radical induced oxidation of tyrosine has been extensively studied and documented [2]. The oxidation of tyrosine by hydroxyl radical leads to the formation of DOPA and dityrosine. DOPA and dityrosine formed by the oxidation are considered as the marker of "oxidative stress". In this study we have detailed the investigations carried out to understand the role of AuNPs on the tyrosine oxidation by OH radical by experimental and by quantum computational techniques. These studies are of high importance in order to understand the exact mechanism of oxidation of tyrosine and alteration in the yield of DOPA and dityrosine in presence of AuNPs by using steady state radiolysis and pulse radiolysis technique.

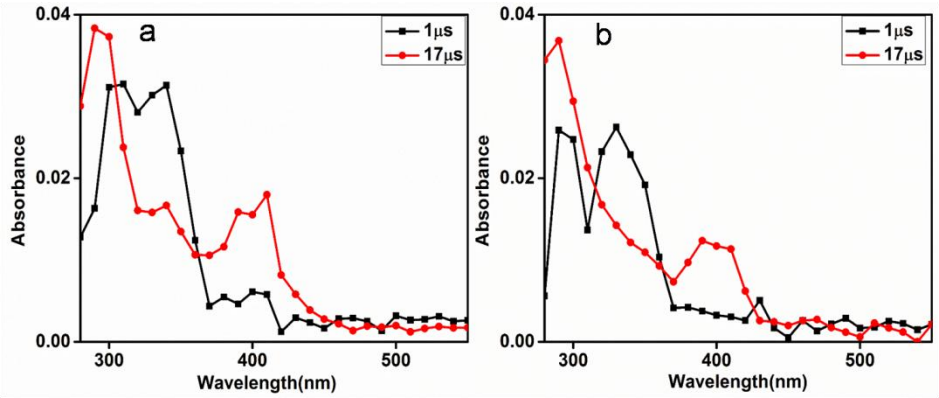

Figure 1: Time resolved transient absorption spectra recorded in the reaction tyrosine with OH radical in a) absence of AuNPs b) Presence of AuNPs.

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Novel Radiation Driven Dynamics in Nanoparticle Sludges

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Radiation induced effects on the interfaces between water and oxides are considered responsible for a variety of anomalous behaviors[1-5]. In certain materials, preferential electron emission from materials into the aqueous during irradiation been observed[3]. This presentation reports on new observations of radiation induced effects in nanoparticle sludges that probe the mechanisms of these interfacial effects.

The first effect is the formation and growth dynamics of hydrogen bubbles in sludges. We have reported the first observation of radiolytic bubble formation[5]. This bubble formation has now been imaged in nanoparticle sludges for a variety of materials, including Al_2O_3, CeO_2, CuO, and Cu_2O, with tomographic scans of each sludge samples undergoing radiolytic bubble formation at different stages in the process. The dynamics of bubble growth are inferred from their changes in bubble shape and size between these scans, giving insight into the underlying dynamics.

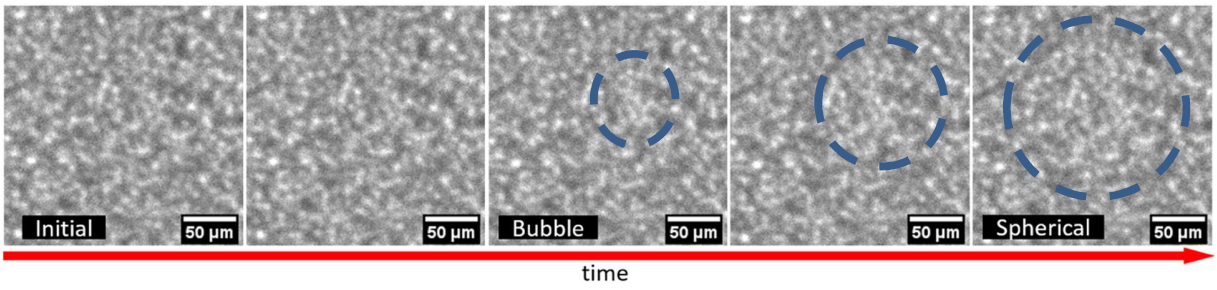

Figure 1. Example of Bubble formation in magnesium hydroxide and water mixture.

The second effect is charge build up within nanoparticles. Radiation induced charge build up has been observed on alumina nanoparticles. In what we believe is another world-first, this charge build up was detected by applying a transverse electric field and observing the deflection of settling nanoparticles during an irradiation. We observed this deflection with x-ray images simultaneously captured from the x-rays transmitted through the sample. The charge-up can be deduced from the angle of deflection observed in these captured images.

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Effects of H_2O_2 speciation in radiation induced dissolution of UO_2-based nuclear fuel

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Interfacial radiation chemistry is of key importance in the development of models to predict the corrosion rate of spent nuclear fuel in contact with groundwater. For the planned final storage in deep geological repositories, both natural and engineered barriers will be utilized to confine the spent nuclear fuel. In an event where the barriers fail, the intrinsic radioactivity of the spent nuclear fuel would induce radiolysis of intruding ground water, resulting in the formation of reactive oxidants ($HO^{\bullet}$, $HO_2^{\bullet}$ and H_2O_2) and reductants (e_{aq}^-, $H^{\bullet}$ and H_2). The oxidative dissolution of UO_2 under deep repository conditions can mainly be attributed to H_2O_2. Although the mechanisms and kinetics of the surface reactions involving H_2O_2 and UO_2 has been studied quite extensively, differences in speciation due to the formation of uranyl peroxo-carbonato complexes had previously not been considered in this context. In this work we assessed the effects of speciation on the kinetics and mechanisms of peroxide consumption and UO_2^{2+} dissolution in 10 mM bicarbonate (pH 8 – 10). The speciation was varied by addition of uranyl nitrate prior to exposure and simulated based on thermodynamic equations using previously reported stability constants[1] and ionic strength correction based on the Specific Ion Interaction Theory model (SIT). It was found that shifting the equilibrium from H_2O_2 towards peroxo complexes significantly (and equally) suppressed both the peroxide consumption and UO_2^{2+} dissolution rates. In additional experiments the formation of surface bound OH-radicals following the decomposition of H_2O_2 on ZrO_2 was studied in the presence and absence of UO_2^{2+}, using Tris(hydroxymethyl)aminomethane (Tris) as a radical scavenger. The detection of formaldehyde in similar yields indicated the same product formed, regardless of speciation. These results are consistent with a peroxide consumption proceeding via the fraction of free H_2O_2 and negatively charged peroxo complex unavailable to the surface. This was supported by the finding that the rates of peroxide consumption for various initial $[H_2O_2]$ can accurately be reproduced based on pseudo-first order kinetics with respect to H_2O_2 when both a relative surface coverage by H_2O_2,[2] and differences in speciation with accumulated exposure is accounted for.

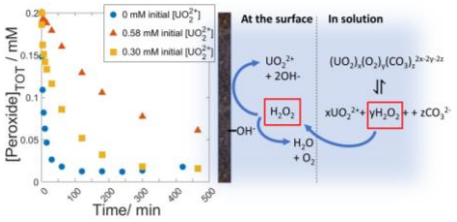

Figure 1. Peroxide concentrations vs time for 50 mg UO_2 powder in 40 mL 10 mM bicarbonate.

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Pulse radiolysis of acetate, malonate and succinate in high temperature water

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Acetate ion (CH_3COO^-) is used in a wide range of applications to scavenge ·OH radicals. This reaction generates the carbon-centered acetate radical ($^{\cdot}CH_2COO^-$) and H_2O by H atom abstraction. The acetate radical can recombine to produce the succinate dianion, which may itself contribute to the overall scavenging process. We have recently studied the reaction of ·OH radical with acetate, succinate and, another polycarboxylic compound, malonate at temperatures up to 350 C, using pulse radiolysis and transient absorption spectroscopy. The transient absorption spectra produced on pulsed radiolysis of N_2O-salturated aqueous solution of acetate and malonate have maxima at 350 nm (ε = 620.0 $M^{-1}cm^{-1}$) and 340 nm (ε = 958.0 $M^{-1}cm^{-1}$) respectively, whereas for succinate, two maxima were observed at room temperature: 290 nm (ε = 798.1 $M^{-1}cm^{-1}$) and 350 nm (688.7 $M^{-1}cm^{-1}$). The reactions of OH radicals with these compounds follow Arrhenius behavior with the activation energy (E_a) 11.1 ± 0.4 kJ/mol and pre-exponential factor (A) of 9.1× 10^9 M^{-1} s^{-1} for acetate; (E_a) 11.9 ± 0.3 kJ/mol and (A) of 17.3× 10^9 M^{-1} s^{-1} for malonate; (E_a) 8.9 ± 0.2 kJ/mol and (A) of 19.7× 10^9 M^{-1} s^{-1} for succinate. One reason for investigating these compounds is to find a useful competition partner to measure other ·OH radical reactions in high temperature water. Generally, our results indicate that acetate presents the best scavenging properties at higher temperatures among the three compounds studied.

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Detecting *superoxide radical anions* in the aqueous medium, resulting from *core-shell ionization* upon exposure to soft X-rays

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Water radiolysis is a widely studied phenomenon, resulting in the formation of reactive oxygen species (ROS) in ionization tracks. These ROS can result in lethal or sub-lethal damage. The *superoxide radical* (HO_2) is one such ROS, generated in heavy ion tracks due to multiple ionization[1,2]. Another pathway of its production is the reaction of electrons with molecular oxygen.[3] However, since this species is biologically toxic, due to its ability to act as a reductant or as an oxidant that might cause major indirect damages, it becomes crucial to investigate it. We, therefore, study the formation of this species following water molecules K-shell ionizations, using theoretical and experimental techniques.

Experimentally, we utilize *soft X-rays (100-1800eV)*, as they offer an advantage of dominant *core-shell ionization*. But, owing to their poor penetration in liquid, there is a scarcity of experimental knowledge in this energy range. Hence, we expose the sample in a microfluidic cell to synchrotron *soft X-rays*.[4] The absorption of photons in liquid water, above the O K edge, results in a doubly ionized water molecule produced after an *Auger relaxation process, surrounded by singly ionized water molecules originating from the photo- and Auger electrons tracks.* Thereafter, the dissociation of the ionized water molecules and intra-track reactions may result in the generation of the HO_2 species, via the reaction $O + OH \rightarrow HO_2$. Superoxide radicals reduce the probe (Water-soluble tetrazole salt, WST8) present in the sample, giving a characteristic signal in the UV, which corresponds to WST8 formazan. The addition of superoxide dismutase (SOD), scavenges the HO_2 species leading to a lowering in reduction hence confirming that HO_2 is one of the causes of this reduction. Performing these experiments in oxic and anoxic conditions, with and without SOD, can help give a better understanding of the various HO_2 formation pathways. *Theoretically*, we simulate the dynamics of a doubly ionized water molecule and a hydroxyl radical in liquid water using Time-Dependent Density Functional Theory and Car Parrinello Molecular Dynamics approaches. The results obtained give an understanding of the production of this species (HO_2), in addition to the formation of H_2O_2.

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Radiolytic Reduction of Li and Mg in Solid Chlorides

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Concerns about climate change are accelerating the development of competitive sustainable energy production technologies. From the available alternatives, molten salt reactors (MSR) meet the characteristics to be a game-changing technology that finally positions nuclear energy (along with wind, hydro and solar) as a viable path towards the decarbonization of the energy sector. In the search for better candidates to function as primary coolant or liquid fuel, it is required to understand the radiation chemistry of complex ionic systems, at different temperature, dose, dose rate, and composition.

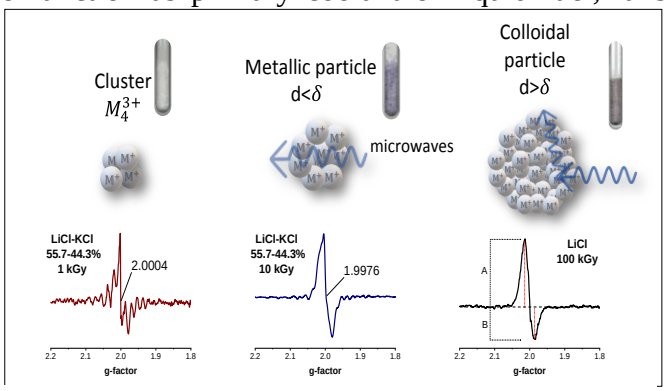

Figure 1. Coalescence of lithium metal atoms induced by gamma radiation in solid chlorides.

The solid-state radiolysis has proven to be a reliable and productive tool to assess primary transients induced by the ionizing radiation in ionic systems, providing fundamental information about speciation and radiation-induced reactivity in chlorides and fluorides with potential applications in MSR's.[1] The evolution of radiation-induced radical species trapped in the crystal, coupled with thermal annealing studies, undoubtedly contributes to elucidate mechanisms of polyhalides and metal particle formation, determinant for the construction of predictive models in molten salts. [2] The present investigation shows studies of Electron Paramagnetic Resonance (EPR) and optical absorption-diffuse reflectance in LiCl and LiCl-KCl (eutectic) powders, as well as KCl-$MgCl_2$ mixtures irradiated with gammas at room temperature. Through the magnetic properties of the metal particles formed, it was possible to monitor the qualitative evolution in size (Figure 1), as well as the radiolytic reduction of Mg in chlorides.

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Radiation induced degradation of fluoroquinolone antibiotics in aqueous solution

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Conventional wastewater treatment plants remove fluoroquinolone antibiotics from wastewater with low efficiency [1]. In this work we show that using the ionizing radiation induced degradation the two investigated fluoroquinolone antibiotics, ciprofloxacin and norfloxacin can be completely eliminated in aqueous solutions. The results showed that 0.5 kGy absorbed dose was sufficient to achieve a percentage removal of more than 70%. Complete elimination needed prolonged irradiation, the antibiotic concentration was lower than the detection limit at 2 kGy absorbed dose. At this dose the degrees of mineralization and oxidation were low (40% and 50%, respectively). Short-lived intermediates (radicals) were studied with the pulse radiolysis technique. Absorption bands of several intermediates were observed on the pulse radiolysis spectra. During the reaction of hydroxyl radical, the build-up of an intermediate with a maximum at 425 nm is seen. During the reaction of hydrated electron, there was a well-separated absorption band with a maximum around 600 nm. The rate constants were 7.2×10^9 mol^{-1} dm^3 s^{-1} and 5.5×10^9 mol^{-1} dm^3 s^- for hydroxyl radical reaction and 8.2×10^9 mol^{-1} dm^3 s^{-1} and 7.3×10^9 mol^{-1} dm^3 s^{-1} for hydrated electron reaction of ciprofloxacin and norfloxacin, respectively. These values are less than an order of magnitude lower than the diffusion controlled limit showing that both diffusion and chemical reactivity have some role in controlling the rate constants [2].

Several degradation products were separated and identified by LC-MS/MS method. Based on their structures the products presumably have no antibiotic effect or have lower antibacterial activity [3]. The main degradation products were hydroxylated variations of the starting compounds, desethylene–ciprofloxacin and –norfloxacin, defluorinated products and anthranilic acid analogues of ciprofloxacin and norfloxacin. Biodegradability was determined from the ratio of biological and chemical oxygen demand values (BOD_{10}/COD). The biodegradability of the original compounds and the degradation products formed at lower doses were very low. Significant increase in BOD_{10}/COD ratio was seen at higher doses, the maximum was at 4 kGy. There is no significant difference between the values obtained for 4 and 6 kGy. The BOD_{10}/COD ratio at 6 kGy was 0.09 and 0.16 for ciprofloxacin and norfloxacin respectively. Based on *Vibrio fischeri* toxicity tests, the early degradation products are more toxic than the initial fluoroquinolones. However, the toxicity decreased by prolonged irradiation. In the case of the antibacterial susceptibility testing the antibacterial activity disappeared parallel with the removal of initial molecules at 2 kGy. The results are in accordance with what was assumed based on the structure of the degradation products.

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The Effects of Electrolytes on the Spectroscopy and Dynamics of Hydrated Electrons

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The hydrated electron has been extensively studied from its generation via photoexcitation or photodetachment through its subsequent relaxation dynamics. However, even though hydrated electrons often occur in ionic environments, such as in batteries or biological cells, there has not been a systematic study on how ionic strength affects the hydrated electron's structure and dynamics. Mostafavi and coworkers examined how the presence of different salts at different concentrations blueshift the absorption spectrum of the hydrated electron,[1] but no hypothesis has been proposed for why the absorption spectrum shifts. Using ultrafast transient absorption spectroscopy and mixed quantum-classical molecular dynamics simulations, we study how non-reactive ions affect both the photodetachment process and the subsequent relaxation of newly-created hydrated electrons. We argue that the blueshift observed in the presence of non-reactive ions is not simply due to the change in dielectric constant induced by the ions, but instead results from ion-induced structural changes of the hydrated electron, including the formation of contact ion pairs with one or several cations. Because contact pairs can form quickly, we also find that the solvent relaxation that follows generation of free electrons in aqueous electrolytes takes place on a similar time scale to that in pure water, despite the significant increase in viscosity and dielectric relaxation time in ionic solutions.

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Radiation-Induced DNA damage and Selective Protection by Antioxidants

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1. INTRODUCTION

Radiation-induced DNA damage can be classified as that produced by direct and indirect actions. *In vitro* experiments on naked DNA samples are expected to clarify the characteristics of DNA damage produced by different radiation actions due to its water content that can be arbitrarily varied. The ratio of water molecules per nucleotide is a key indicator showing that direct and indirect effects play a dominant role in DNA damage at the ratios less than 40 and greater than 1000, respectively. Besides, additives such as antioxidants can selectively reduce a certain type of radiation-induced DNA damage. In the pulse radiolysis experiment, the antioxidant rutin was found to remove oxidizing radicals, •OH (radical scavenging) and to repair unstable oxidative DNA damage (chemical repair) [1]. This study reports partial progress on stable DNA damage induced by direct or indirect radiation actions and the selectively protective effect of antioxidants.

2. EXPERIMENT

The methods of extraction and purification of DNA sample (Plasmid DNA, pUC18) are described elsewhere [2]. Film [3] and solution DNA samples without any buffer solutes were prepared and irradiated with X-rays (160 kVp, 3 mA) for detecting damage induced by direct and indirect actions, respectively. Agarose gel electrophoresis quantified the single-stranded breaks (SSBs), double-strand breaks (DSBs), and base lesions. The simulation code PHITS corrected for the effect of the structure of the DNA sample on the absorbed dose.

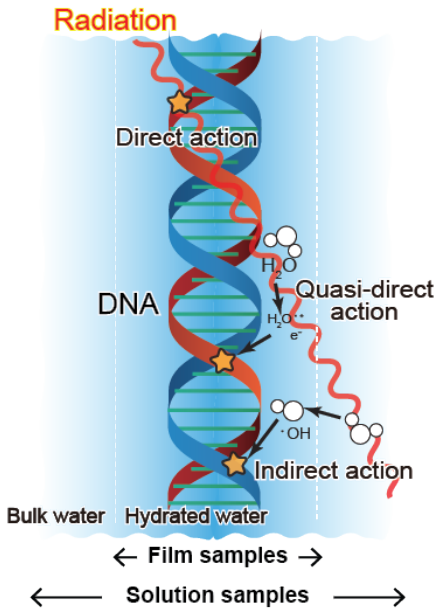

Fig. A schematic diagram of different types of radiation-induced DNA damage and their detection.

3. RESULTS & DISCUSSIONS

The yields of SSBs, DSBs, and base lesions in solution were higher than those in film samples. This is because the high content of water molecules produces more •OH that can cause DNA damage in solution samples. In addition, isolated base lesions and DSBs were found frequently in film samples, while cluster damage, including base damage, was much common in solution samples. This result is attributed to the different locations of energy transfer from radiation to DNA. Besides, the yields of SSB and DSB in this report were about 10 times higher than those reported using TE buffer [3], but the yields of base lesions were only about 2.6-6.5 times higher. The variation in the yield of these damage types suggests that the •OH scavengers, such as Cl^- and Tris in the TE buffer, were selective in the protective effect of DNA damage.

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Grafted mesoporous silicas for radionuclide uptake: radiolytic stability under electron irradiation

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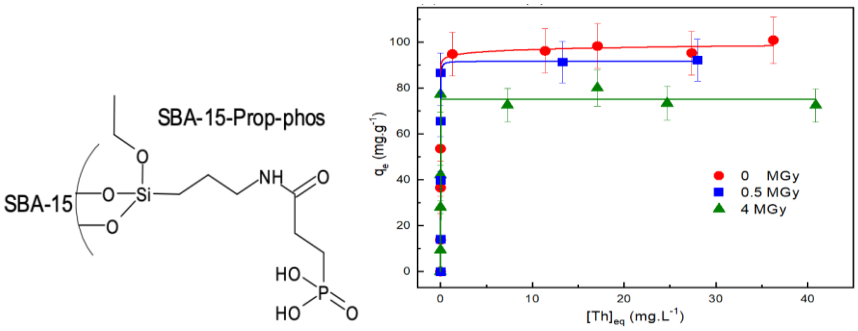

Figure 1. Left: Structure of the SBA-15 material grafted with the propionamide phosphonate ligand (SBA-15-Prop-phos). Right: Adsorption isotherms of Th using SBA-15-Prop-phos before (0 MGy) and after irradiation at 0.5 MGy and 4 MGy.

Mesoporous silicas grafted with organic ligands were found to be useful tools for the capture of radionuclides from aqueous streams [1]. However, materials developed for radionuclide adsorption need to be robust against ionizing radiation. In this work, we evaluated the degradation of mesoporous silicas (SBA-15) grafted with hydroxypiridinone, acetamide and propionamide phosphonate ligands under electron irradiation. Materials were irradiated up to 4 MGy, and characterized by means of FT-IR, XPS, TGA and gas measurements techniques. Irradiation led to the degradation of the amide functional group and to the production of amine and carboxylic acid groups, as already observed during the irradiation of amide-containing ligands [2]. Corresponding reaction mechanisms were proposed. The sorption behavior of the grafted SBA-15 materials for thorium was also studied (see the adsorption isotherm of Th with SBA-15-Prop-phos before and after irradiation in Figure 1). The propionamide phosphate ligand was shown to be the most efficient, with an equilibrium sorption capacity of 95 mg·g^{-1}. This capacity remained stable up to a 1 MGy and decreased by 20% after an irradiation of 4 MGy. Therefore, this material is potentially interesting for application in the decontamination of nuclear power plant cooling systems for which it could be used for at least 10,000 hours (~14 months, [3]) without any change in its sorption ability.

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C_2H_2···CO complex and its radiation-induced transformations: a building block for cold synthetic astrochemistry

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Model matrix-isolation studies on the radiation chemistry of astrochemically relevant molecules are very useful for a better understanding of the radiation chemistry occurring in cold space media [1]. Acetylene (C_2H_2) is one of the simple molecules known to occur in various extraterrestrial environments (particularly, in cometary ices), mainly as an admixture to principal components, such as CO [2]. Thus, one may expect that the acetylene complex with CO may be considered as an important building block for complex organic molecules and biomolecules in space. In a wider context, the impact of weak intermolecular complexes may present general interest for basic radiation chemistry. In this work, we have examined the low-temperature radiation-induced transformations of the 1:1 C_2H_2···CO intermolecular complex using matrix-isolation approach using FTIR and EPR spectroscopy [3, 4] complemented with theoretical studies at the UCCSD(T) level of theory.

Matrix samples were obtained by deposition of gaseous mixtures (C_2H_2/CO/Ng 1/3/1000; Ng = Ar, Kr, Xe) onto a cold KBr substrate mounted in a closed-cycle helium cryostat. The conditions of the deposition procedure were optimized to obtain a sufficient amount of the precursor 1:1 C_2H_2···CO complex. The deposited matrices were irradiated with X-rays (effective energy ca. 20 keV) to different doses (up to 200 kGy) at 5 K. Photolysis of the irradiated samples was performed using appropriate LEDs (λ_D = 465 nm and λ_D = 410 nm). The radiation-induced products and intermediates were characterized by FTIR and EPR spectroscopy.

It was found that the X-ray radiolysis of the low-temperature noble gas matrices containing 1:1 C_2H_2···CO complex resulted in the formation of C_3O (tricarbon monoxide), HCCCHO (propynal), c-H_2C_3O (cyclopropenone), H_2CCCO (propadienone), and $HC_3O^{\bullet}$ (oxoprorynyl radical) at 5 K. Remarkably, the observed transformations of the complex represent synthetic routes leading to various C_3 species, whereas the acetylenic C–H bond cleavage yielding ethynyl radical appears to be a minor process. Prolonged irradiation results in dehydrogenation, while the C_3 skeleton is retained. IR and EPR spectroscopic studies supported by extensive *ab initio* UCCSD(T) calculations revealed the formation of a particular isomer of the $H_2C_3O^{+\bullet}$ radical cation as a key reactive intermediate. The interpretation of the C_2H_2···CO radiolysis mechanism (possible reactions pathways) is given based on the analysis of kinetic curves and matrix effect.

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One-pot radiation-induced preparation of metal–polymer nanocomposites in aqueous solutions of 1-vinyl-1, 2, 4-triazole containing silver ions

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The unique functional properties of materials based on metal-polymer nanocomposites have been stimulating interests in the methods to their synthesis over the past three decades [1]. General approach for preparation of nanoparticles is the reduction of metal ions in solutions in the presence of a suitable polymer matrix. However, in recent years, great efforts have been paid to the development of methods for the production of nanocomposites, in which the synthesis of metal nanoparticles and the formation of a stabilizing matrix occurs in one reactor. In this regard, specific attention has focused on the radiation-chemical approach [2], which can provide the opportunities for obtaining various metal-polymer systems, for instance, soluble composites, dense and weakly cross-linked gels.

In this work, we report on the synthesis of silver nanoparticles (AgNPs) stabilized by poly(1-vinyl-1, 2, 4-triazole) (PVT) in aqueous solutions of 1-vinyl-1,2,4-triazole (VT) containing silver ions due to the processes of radiation-induced polymerization and the assembly of AgNPs. The kinetics features of the polymerization and formation of AgNPs have been studied using UV-Vis spectroscopy. TEM-data show the generation of relatively small AgNPs with an average size of 2-3 nm and a narrow size distribution, which indicates the effective stabilization of nanoparticles by triazole units. Gel permeation chromatography data exhibit an increase in PVT molecular weight with increasing monomer concentration. At the same time, the addition of ethanol suppresses the crosslinking of macromolecules in solution. The results obtained demonstrate that aqueous–alcoholic solutions of 1 wt.% VT can be used to obtain soluble nanocomposite materials, while 10 wt.% monomer solutions have prospects for use in the preparation of polymer gels filled with nanoparticles [3].

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EARLY CAREER SCIENTIST FLASH PRESENTATIONS

All the flash presentations have an associated poster in the poster session

Comparison of transient Raman spectra of hydrated dimer radical cations of thiourea and selenourea

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Time-resolved Raman spectra of the dimer radical cations of thiourea, $(Tu)_2^{\bullet+}$, and selenourea, $(Su)_2^{\bullet+}$, prepared by pulse radiolysis of N_2O saturated aqueous solutions of thiourea (Tu) and selenourea (Su) , respectively, were obtained in resonance with their transient optical absorptions using 415 nm excitation wavelength. We interpreted spectra in conjunction with theoretical calculations to provide detailed information on the molecular geometry and bond properties of the studied species, find their similarities and point out apparent differences.

Time-resolved resonance Raman spectra of both radical dimer cations recorded in the spectral range of 70-900 cm^{-1} have apparent pseudo-diatomic nature with strongly enhanced fundamental bands at 137 and 212 cm^{-1}, which are assigned to symmetric stretch of Se-Se and S-S hemibonds, respectively. From progression of overtones of these fundamental vibrations bond dissociation energies of 1.21 and 1.25 eV, respectively, have been obtained using Birge-Sponer extrapolation, further supporting assignment of a hemi-bonded nature of the mainly enhanced oscillators. Unlike in $(Su)_2^{\bullet+}$, additional very weakly enhanced band located at 719 cm^{-1}, which combines with 212 cm^{-1} fundamental is apparent in $(Tu)_2^{\bullet+}$ spectrum, and based on theoretical predictions can be assigned to C-S symmetric vibration in $(Tu)_2^{\bullet+}$. Upon substitution of labile protons of $(Tu)_2^{\bullet+}$ with deuterons in D_2O solutions frequencies of fundamental vibrations observed in H_2O decrease to 208 and 668 cm^{-1}, respectively, and two additional fundamentals become apparent at 380 and 410 cm^{-1} overlapping with first overtone of 208 cm^{-1} band. Following theoretical studies these bands can be assigned to SCN in phase bending and NCN symmetrical deformation, respectively. On the contrary, resonant Raman spectra of $(Su)_2^{\bullet+}$ do not show any noticeable change in D_2O solutions.

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Multiscale Modeling of the Radical-Induced Chemistry of Acetohydroxamic Acid in Aqueous Solution

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Acetohydroxamic acid ($CH_3CONHOH$, AHA) is a small organic acid with several pharmacological and industrial applications that make use of its ability to strongly chelate metals, including proposed use in spent nuclear fuel reprocessing cycles. In these applications, AHA may interact with free radical species in a variety of environments, which necessitates a fundamental understanding of the degradation behavior of AHA to predict and control these processes. To this end, we present a comprehensive, multiscale computer model for interrogating the radical-induced degradation of AHA in aqueous solutions. Model predictions were critically evaluated by a systematic experimental radiation chemistry investigation, leveraging pulsed electron techniques for the measurement of new radical reaction rate coefficients, and steady-state gamma irradiations for the identification and quantification of AHA degradation products. Excellent agreement was achieved between calculation and experiment, indicating that this fundamental model can accurately predict the degradation pathways of AHA in aqueous solutions under relevant conditions.

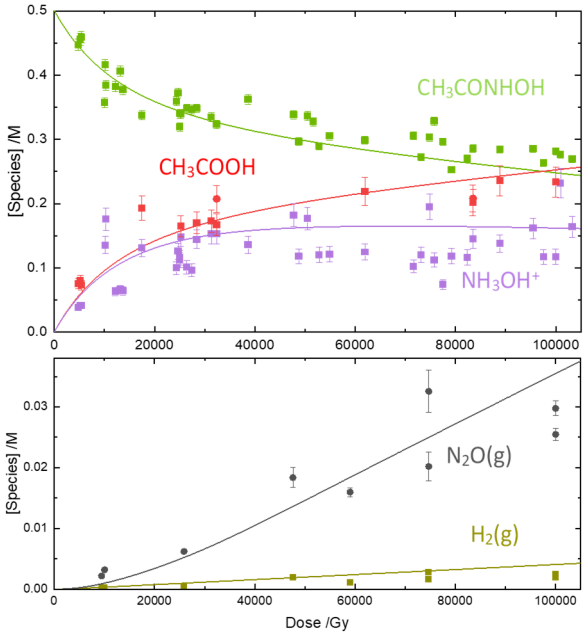

Figure 1. The loss of 0.50 M $CH_3CONHOH$ in 0.20 M HNO_3 as a function of absorbed gamma dose at 40 °C and the in-growth of its degradation products: CH_3COOH, NH_3OH^+, $H_2(g)$, and $N_2O(g)$. The experimental data points are from UV-visible spectroscopy, gas chromatography, and ion chromatography, and the curves are predicted values from the multiscale model.

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CH_3CN complexes with water and carbon dioxide and their radiation-induced transformations in low-temperature matrices

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Small nitrogen-containing molecules play an important role in extraterrestrial prebiotic chemistry. In particular, acetonitrile (CH_3CN) was found in different space objects [1, 2]. It is supposed to be a precursor of a variety of biologically relevant molecules, including amino acids [3, 4]. Considering the solid-phase chemistry driven by ionizing radiation, one may come to an idea that the intermolecular complexes of acetonitrile with oxygen-bearing molecules can serve as "building blocks" for complex organic molecules (COMs) containing both N and O atoms. However, little is known on the mechanisms of such processes. The strategy to investigation of the radiation-chemical transformations occurring within isolated complexes frozen in rigid environment was recently developed in our laboratory [5, 6]. In this work we have examined for the first time the radiation-induced transformations of acetonitrile complexes with the most common space molecules (water and carbon dioxide) occurring under X-ray irradiation in solid argon matrices at 5 – 6 K using FTIR spectroscopy.

As a first step, the 1 : 1 and 1 : 2 complexes of acetonitrile with water were experimentally obtained by condensation of the ternary gaseous mixtures ($CH_3CN/H_2O/Ar$) and characterized on the basis of comparison with available computational data [7]. Then, it was shown that the radiolysis of complexes with X-rays led to formation of oxygen-containing COMs, such as acetamide, hydroxyacetonitrile and glycine. The formation of these products was also confirmed by experiments with isotopic substitution (CD_3CN). Remarkably, the simplest amino acid (glycine) was detected almost immediately after irradiation at 5 K, which may indicate a new route to the cold radiation-induced synthesis of this important prebiotic molecule in the space environment.

The complex of acetonitrile with CO_2 was identified after deposition of $CH_3CN/CO_2/Ar$ (1/1/1000) sample. Its radiation-induced decomposition results in formation of a relatively small amounts of oxygenated molecules, but glycine was not found in this case. Possible mechanisms of the radiation-chemical processes and astrochemical implications of the results are discussed.

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Bragg's Additivity Rule and Core and Bond model of water vapor studied by real-time TDDFT electronic stopping calculations

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The electronic stopping power (S_e) for protons in water vapor (H_2O), hydrogen (H_2) and oxygen (O_2) gases was calculated in a broad range of energies around the Bragg peak, using real-time TDDFT simulations with Gaussian basis sets. This was done for a kinetic energy of incident protons (E_k) ranging from 1.56 keV/amu to 1.6 MeV/amu. S_e was calculated as the average over geometrically pre-sampled short proton trajectories. The average $S_e(E_k)$ values were found to rapidly converge with 25-30 pre-sampled, 2 nm-long trajectories. The rt-TDDFT $S_e(E_k)$ curves were compared to experimental and SRIM data, and used to validate the Bragg's Additivity Rule (BAR). Discrepancies were analyzed in terms of basis set effects and omitted nuclear stopping at low energies. At variance with SRIM, we found that BAR is applicable to our rt-TDDFT simulations of $2H_2+O_2 \rightarrow 2H_2O$ without scaling for E_k>4 keV/amu. Analyzing the Core and Bond (CAB) approach, where the contribution to stopping is divided into that of the unchanged atomic core and that of binding electrons, we found that the CAB contributions of H and O to S_e were slightly smaller than SRIM values as a result of a red-shift in our rt-TDDFT $S_e(E_k)$ curves and a re-distribution of weights due to some bond contributions being neglected in SRIM.

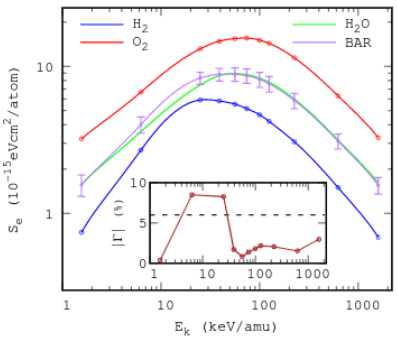

Figure 1. The BAR additivity of rt-TDDFT S_e, according to $2H_2+ O_2 \rightarrow 2H_2O$. The inset shows the relative scaling factor Γ obtained from rt-TDDFT (brown dots), along with the constant scaling value recommended by SRIM (dashed line).

Table 1. Hydrogen and oxygen related CAB contributions to S_e calculated by rt-TDDFT simulations and SRIM-2013. The unit of stopping power is 10^{-15}eVcm^2/(atom or bond). The last column reports the relative percentual difference between rt-TDDFT and SRIM.

	Name	rt-TDDFT	SRIM-2013	ϵ(%)
Core	H	0	0	0
	O	4.68±0.35	5.36	-12.6
Bond	H-H	8.46±0.61	10.049	-15.8
	H-O	9.37 ± 0.77	10.085	-7.1
	O-O	5.1±1.27	–	–
	O=O	19.24±1.43	22.044	-12.6

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Effect of electron beam irradiation and the presence of antibiotics on the population dynamics of resistant/sensitive bacterial cultures in model wastewater matrix

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Control strategies against the spread of antibiotic resistance should be considered in wastewater treatment plants. It is important to understand how resistant bacteria behave in the presence of trace amounts of antibiotics, in order to implement appropriate measures. It should be also considered too that the species present in these diverse microbial populations show different sensitivities to irradiation [1]. In this work, we examined the population dynamics of resistant/sensitive Staphylococcus aureus co-cultures. On the one hand, we gained insight into the effect of trace amounts of antibiotics (piperacillin and erythromycin) on bacteria in different wastewater matrices, and on the other hand, we studied the applicability of electron beam (EB) irradiation to eliminate the antibacterial effect. Based on our results, we suggest that trace amounts of antibiotics has an effect on the resistant strain. Presumably, irradiation triggers biological processes in resistant bacteria that do not provide a competitive benefit but disadvantage over the sensitive subtype, and the trace level of the antibiotic present does not appear to affect the sensitive strains. The effect of these conditions on population dynamics is reduced with the use of EB, presumably due to the fact that the decomposition products of the components of the effluent matrix (such as humic acid) also contribute to the chemical transformations. Furthermore, it has become apparent that the presence of trace amounts of antibiotics initiates biochemical processes in the resistant subtype, besides, it sensitizes bacteria to the attack of free radicals generated during EB treatment. It is clear that the effects of trace level of antibiotics in environmental waters on the cellular response and population behavior of resistant bacterial cultures deserves more detailed studies.

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Exploring Physical and Chemical Effects of Radiation on Explosives

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High explosives can be found in a variety of applications that involve ionizing radiation fields, though the challenges associated with conducting such experiments have resulted in very few investigations into the radiation aging of explosives. Recent results observe that the handling sensitivity, or the ability of an explosive to initiate under typical handling scenarios, can dramatically increase following irradiation. [1-4] Chemical analyses following irradiation suggest that much of the damage is located on the energetic functional groups that give molecules their explosive properties. [5] The removal of energetic functional groups, such as the transformation from pentaerythritol tetranitrate (PETN) to pentaerythritol trinitrate (PETriN) as shown in Fig. 1, leads to a decrease in sensitivity, however. One theory postulated that the radical species generated during irradiation could be responsible for the increased sensitivity, but that theory was shown to be incorrect. [1] The reason for the increase in sensitivity of explosives following irradiation is still not known.

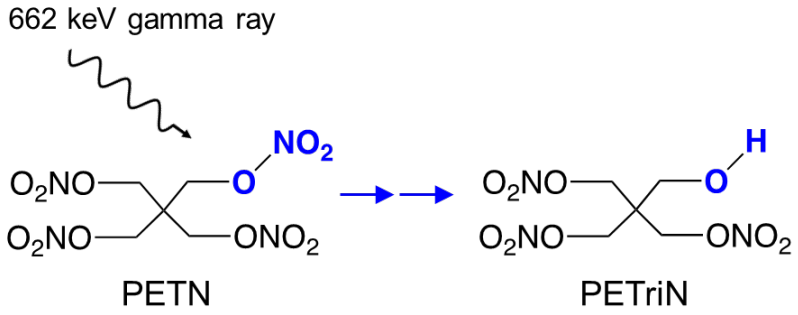

Figure 1. Simplified scheme showing the primary observed radiolytic decomposition product of PETN.

This talk will discuss what is currently known about radiolytic decomposition of energetic materials and the relationship between radiation aging and the sensitivity of explosives as well as planned future experiments to further the investigation into this topic.

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Computer simulated degradation of $CFCl_3$ under electron beam

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Chlorofluorocarbons are atmospheric reservoirs for Chlorine in the atmosphere. They catalyze the destruction of Ozone by releasing chloride atoms therefore indirectly having adverse environmental implications. Chlorofluorocarbons, as is common with halogen containing compounds have excellent affinities for electrons. Electron beam irradiation has been shown to be a versatile method in the destruction of various organic molecules including Chlorofluorocarbons. The interaction of radiation with the gaseous matrix causes the production of reactive species that facilitate the decomposition of organic molecules within it. Dissociative electron attachment has been shown to be one process that propagates the degradation of chlorofluorocarbons under electron beam irradiation. Additionally, reactions with Hydroxyl radicals and Oxidation processes facilitate further destruction.

Computer simulations are effective tools in predicting the efficacy of EBT for removal of organic compounds. From simulations it is possible to predict the main decomposition reaction pathways and the major products formed . It also provides a framework for testing different parameters and conditions that would enhance the chemical process. A scheme for the destruction of single carbon chlorofluorocarbon under electron beam irradiation in synthetic air (80% N_2, 20% O_2) will be presented. The effects of dose rate, effective dose, water concentration, oxygen concentration on the overall removal efficiency will also be presented

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Radiation induced dissolution of studtite and meta-studtite

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Studtite and meta-studtite are the only known uranyl peroxide minerals in nature. The precipitation of studtite in solutions containing sufficient concentrations of hedrogen peroxide (H_2O_2) and uranyl (UO_2^{2+}) occurs at a temperature below 50 °C, while meta-studtite precipitates at a temperature above 70 °C. Both of them have very low solubility in H_2O. However, as carbonate enables the formation of soluble uranyl-carbonate and uranyl-peroxo-carbonate complexes, the rate of meta-studtite and studtite dissolution are expected to increase with increasing carbonate concentration. In this work, we studied the dissolution of studtite and meta-studtite in 10 mM HCO_3^- solution with and without the gamma-irradiation. The uranyl species formed during the dissolution process were characterized using ^{13}C-NMR. It is found that studtite and meta-studtite dissolve in HCO_3^- solutions through the formation of uranyl-carbonato and uranyl-peroxo-carbonato complexes, and meta-studtite is considerably more soluble than studtite. Moreover, in the presence of gamma-irradiation, both studtite and meta-studtite dissolve much faster than without gamma-irradiation. Furthermore, as studtite and meta-studtite dissolve more UO_2^{2+} than H_2O_2 in general, we performed additional H_2O_2 stability experiment. It is shown that H_2O_2 is catalytically decomposed in solutions containing UO_2^{2+} and HCO_3^- with an optimum UO_2^{2+} concentration.

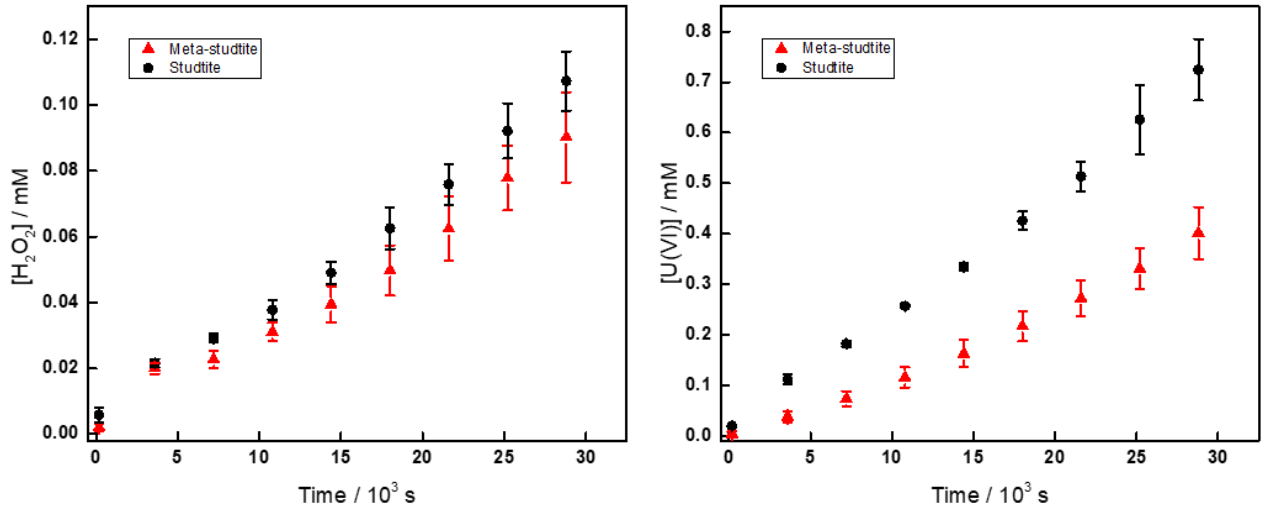

Figure 1. Concentration of H_2O_2 (a) and U(VI) (b) as a function of time for irradiated aqueous meta-studtite (red triangles) and studtite (black dots) powder suspensions containing 10 mM HCO_3^-.

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Radiation-induced assembling of benzene and naphthalene molecules from molecular aggregates and complexes at low temperatures

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The origin of polycyclic aromatic hydrocarbons (PAHs) in space presents a great challenge for astrochemistry since the first observations of these species in the interstellar medium [1,2]. According to one of the proposed hypotheses, PAH structures can result from small hydrocarbon molecules in cold space regions due to the radiation-induced synthesis occurring in the absence of molecular mobility, which generally implies an important role of molecular organization. However, the mechanisms of such "molecular assembling" are still unclear and the nature of possible precursors of PAHs in the solid phase is under discussion. In this work we have first experimentally tested the possibility of the radiation-induced synthesis of benzene and naphthalene molecules from molecular aggregates and complexes in rigid environment using noble gas matrices as model media.

An original closed-cycle helium cryostat cryocooler was used in experiments. The gas mixtures containing precursor molecules and excess amount of noble gas (Ar, Kr, or Xe) were deposited onto a cooled KBr substrate at 12–40 K and irradiated with X-rays at 6 K. The radiation-induced transformations were monitored by FTIR spectroscopy at 6 K.

In the case of benzene [3], acetylene was used as a precursor. The solid C_2H_2/Ng (1:300) samples containing sufficient amounts of the $(C_2H_2)_3$ aggregates were obtained by adjusting the deposition conditions and characterized by specific spectroscopic signatures. It was demonstrated that a benzene molecule could be directly produced from the trimer after irradiation at 6 K, which implies a single-step process without formation of any detectable intermediates.

In the case of naphthalene, we tried to use several precursors such as $C_6H_5C_2H_3…C_2H_2$, $C_6H_5CCH…C_2H_2$, and $C_6H_5CCH…C_2H_4$ molecular complexes isolated in the noble gas matrices. Somewhat unexpectedly, it was found that only the former complex yielded naphthalene after irradiation at 6 K [4]. Additional experiments with electron scavenger (SF_6) revealed that the assembling of neutral naphthalene molecule probably occurs through the formation of naphthalene radical cation, which strongly supports a cationic pathway. Possible mechanisms of reactions and astrochemical implications are discussed.

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Effect of biomolecule environment on the energy deposition of swift charge particles by first principles simulations.

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When swift ionic particles penetrate in biomolecules, in a few attoseconds, they deposit some of their energy by Colombian interaction between charge particle and electron cloud of biomolecule. Accurately quantifying the deposited energy is essential in many fields of science for instance astrophysics, nuclear material, nuclear medicine. The mechanism of energy transfer initiates when a positively charged particle encloses the electron cloud of the target martial, drags and strongly polarizes the electrons clouds, the electron density accumulates on the impacting molecular fragment and partially reduces on surrounding molecular fragments [1]. According to this mechanism, the cooperativity of environment molecules could influence the energy deposition (collective effect). It is generally considered that energy deposition is a local process which is little influences by the molecular environment.

In order to estimate the effect of the surrounding molecular fragments on the energy deposition (collective deposited energy), we irradiated a supramolecular system and isolated molecular fragments of it by swift proton with difference kinetic energy. The simulations have been done by means of numerical electron dynamic model *real-time time dependent auxiliary density functional theory* (RT-TD-ADFT) [2] which successfully calculates the deposited energy in time real as promising model. We reveal that the quantity of collective deposited energy is significant in our system, it varies from 5% to 12% with respect to the kinetic energy of the proton. In addition, the contribution of collective effect comes from the long- distance interaction of electric field of charge particle. this interaction reduces at low velocity due to the screening of electric field of charge particle by accumulation of electron density around it.

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Reactions of the radiation-induced oxygen atoms with fluoroform and its radiolysis products: a model matrix isolation and ab initio study

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Reactions of atomic oxygen with chemically inert molecules present considerable interest for atmospheric chemistry, gas-phase kinetics, and chemical dynamics. Considering the modern ecological challenges, one should pay special attention to fluoromethanes (CH_2F_2 and CHF_3), which are widely used as an alternative to chlorinated freons supposed to be responsible for the depletion of the ozone layer. Indeed, in contrast to chlorinated analogs, CH_2F_2 and CHF_3 are chemically and photochemically stable, but they can be activated by ionizing radiation or reactions with oxygen atoms produced from highly abundant atmospheric compounds. The radiation chemistry of isolated CHF_3 and CH_2F_2 molecules and some of their atmospherically relevant complexes was recently investigated in our group using a matrix isolation approach [1–3]. As a next step, we applied this approach to simulate the reactions of fluoroform and products of its degradation with "hot" and thermal O atoms, which could be crucially important for the evolution of this compound in upper atmospheric layers, using different sources of O atoms.

In the present work, we report an experimental and theoretical study on the radiation-induced and post-irradiation thermal reactions occurring in the $CHF_3/N_2O/Ng$ or $CHF_3/H_2O/Ng$ (Ng = Ar, Xe) systems irradiated with X-rays at 6 K. It was found that two products of the fluoroform oxidation were stabilized under these conditions: COF_2 and its intermolecular complex COF_2…HF. The latter species (a hydrogen-bonded complex) was first characterized in this work on the basis of a comparison between theoretical and experimental complexation-induced shifts in the IR spectra. The reaction pathways were analyzed from the theoretical point of view on the basis of consideration of potential energy surface (PES). Generally, there are two possible channels, corresponding to the insertion of oxygen atoms into C-H or C-F bonds. It appears that both channels exhibit a significant barrier, which can be overcome only due to involvement of "hot" oxygen atoms produced upon the radiolysis of oxygen-containing precursor molecules. Indeed, according to the experimental results, the oxidation products were produced only in the course of radiolysis and they were not formed upon annealing at appropriate temperatures when the trapped oxygen atoms become thermally mobile. In addition, we have found an indication of the reactions between $O(^1D)$ atoms and fluoroform radiolysis products, such as CF_2 and CF_3.

The implications of the results for atmospheric chemistry are discussed.

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The influence of H/D kinetic isotope effect and structure of α-diols on their radiation-induced fragmentation in deaerated aqueous solutions

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For the investigation of radiation-induced free-radical biomolecule damage vicinal diols and their derivatives as model compounds can be exploited. These low molecular weight compounds contain similar structural parts to hydroxyl-containing biomolecules such as carbohydrates, phospholipids, ribonucleotides, amino acids and peptides. This work is devoted to a more complete study of free radical transformations of such biomolecules and to search for new approaches to regulation of such processes.

The obtained values of the radiation-chemical yields of the products of the studied compounds allow us to conclude that α-diols with a terminal position of hydroxyl groups (propane-1,2-diol, butane-1,2-diol) undergo free radical fragmentation by a chain mechanism (Figure 1). The key role in chain continuation is played by a reactive terminal carbon-centered radical. In the case of medial position of hydroxyl groups (butane-2,3-diol), a similar dehydration mechanism does not occur due to the formation of a more stable secondary carbon-centered radical.

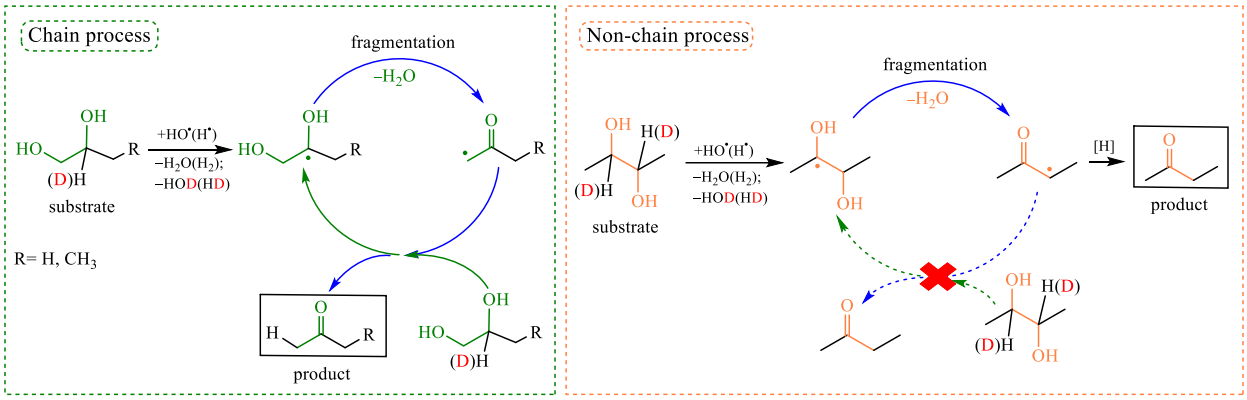

Figure 1. Schemes describing the indirect radiolysis of propane-1,2-diol, butane-2,3-diol and their deuterated analogues as well as butane-1,2-diol in deaerated aqueous solutions.

The studies clearly indicate that the chain nature of the radiation-induced formation of acetone in propane-1,2-diol deaerated aqueous solutions is quenched by replacing hydrogen with deuterium in position C_2 of the initial compound. The exceptional role of primary β-carbonyl radicals in the radiation-induced chain dehydration of diols and, as a result, in the appearance of a strong kinetic isotope effect, is also demonstrated by the absence of a kinetic isotope effect when butane-2-one is formed from butane-2,3-diol or butane-2,3-diol-2,3-d_2 in deaerated aqueous solutions.

Radio-grafting of phosphorus flame retardant on flax fabrics: Pre-irradiation method

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This work is focused on the functionalization of flax fibers aiming to improve their flame retardancy by grafting a phosphorus-based flame retardant (FR), dimethyl(methacryloxy) methyl phosphonate (MAPC1). The pre-irradiation method [1], [2] was used, and the grafting process follows three main steps namely: the irradiation of flax fibers, the impregnation of irradiated fibers in FR solution and finally a washing step to remove unreacted monomer units and free oligomers and polymers chains not covalently bonded to the flax structure. The presence of radicals on the flax fibers after irradiation was confirmed by Electron Paramagnetic Resonance. Grafting efficiency was assessed by infrared spectroscopy and quantified using Inductively Coupled Plasma. The location of the grafted phosphorus polymer chains was assessed by Scanning Electron Microscope coupled with Energy Dispersive X-ray spectrometer using phosphorus mapping of modified fibers. The effect of phosphorus grafting on thermal properties and fire behavior of flax fibers was studied using thermogravimetric analysis, pyrolysis combustion flow calorimetry and cone calorimetry. Different parameters were studied such as the radiation dose, the temperature and the duration of the grafting reaction and the monomer concentration. In particular, it was observed that MAPC1 was grafted in a homogeneous way into the bulk of the elementary flax fibers leading to high phosphorus rate of around 2 wt% for a dose 10 kGy and up to 7 wt% for a dose 100 kGy leading to high charring and low flammable fibers.

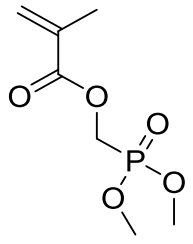

Figure 1. Chemical structure of MAPC1.

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Radiation-chemical synthesis of C_2 and C_3 nitriles in cryogenic media

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The CN containing molecules are important astrochemical species, which occur in interstellar and other extraterrestrial media and probably play a significant role in prebiotic chemistry [1]. In this work, we have first demonstrated the formation of a number of C_2 and C_3 nitriles and isonitriles from the 1:1 CH_4···HCN and C_2H_6···HCN complexes in the low-temperature matrices.

The parent complexes isolated in a noble gas (Ng) matrix were obtained by deposition of the CH_4/HCN/Ng and C_2H_6/HCN/Ng gaseous mixtures. Characterization of the complexes was performed by comparison of the HCN infrared absorption band experimental complexation-induced shifts with the results of the ab initio calculations [2]. The deposited samples were irradiated with X-rays (effective energy ca. 20 keV) to different absorbed doses (up to 300 kGy) at 6 K. The radiation-induced products and intermediates were identified by FTIR spectroscopy.

It was found [3] that the X-ray irradiation of low-temperature matrices containing the isolated CH_4···HCN complexes results in the formation of acetonitrile (CH_3CN) and isoacetonitrile (CH_3NC) and it appears to be the first experimental evidence for the formation of C_2 nitriles from such a "building block". Additionally, a CH_4···HNC complex was tentatively assigned in the irradiated Ar and Kr matrices. It was demonstrated that the matrix has a strong effect on the CH_3CN/CH_3NC yield ratio, which dramatically increases in the row Ar < Kr < Xe. Also, the efficiency of the CH_4···HNC complex radiation-induced formation decreases from Ar to Kr.

The radiation-induced transformations occurring in the C_2H_6/HCN/Ng systems [4] results in the formation of C_2H_3CN, C_2H_3NC and C_2H_5NC. In addition to synthetic products (C_3H_xN molecules), irradiation results in dehydrogenation of the initial complexes and their isomerization to the corresponding HNC···C_2H_n complexes. The formation of propionitrile (C_2H_5CN) also cannot be excluded, although this molecule was not detected experimentally, possibly due to its poor infrared absorption coefficients. Cyanoacetylene (HC_3N) is accumulated with an induction period and becomes predominating at high absorbed doses, which points to its formation from the radiation-induced dehydrogenation of the primary products. The obtained results suggest new possible routes for formation of nitriles, isonitriles and cyanoacetylene in complex astrochemical ices.

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γ-Radiation-Induced Hydroxylation on Boron Nitride Nanosheets for Selective Oxidative Dehydrogenation of Propane

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Hexagonal boron nitride (*h*-BN) is a promising catalyst for selective production of propylene *via* oxidative dehydrogenation of propane (ODHP).[1] Modification of *h*-BN with hydroxyl groups can improve the catalytic performance.[2] However, high thermal and chemical inertness of *h*-BN hinder the functionalization. Here, we achieved the efficient hydroxylation of *h*-BN nanosheets (BNNSs) by γ-irradiation in N_2O-saturated aqueous suspension. Porous BN (**PBN**), the precursor of BNNSs, were synthesized *via* Chemical Blowing.[3] **PBN** were sonicated or γ-irradiated in aqueous solution to obtain BNNSs, of which the products were termed as **BNNS-S** and **BNNS-R**, respectively. The attenuated total reflectance-Fourier transform infrared (ATR-FTIR) spectra demonstrated that **BNNS-R** had a much higher hydroxylation degree than **BNNS-S** (**Figure 1a**). The percentage of B–O component dramatically rose to 38.3% (**Figure 1b** and **1c**). Pulse radiolysis verified that the reaction between BNNSs and $^{\bullet}OH$ played a crucial role in the hydroxylation, of which the rate constant k was 2.6×10^7 L g^{-1} s^{-1} (**Figure 1d**). In comparison with other BN materials, **BNNS-R** performed a high propylene selectivity of 75% at a high propane conversion of 14% (**Figure 1e**), which overcame the contradictory between high selectivity and high conversion.

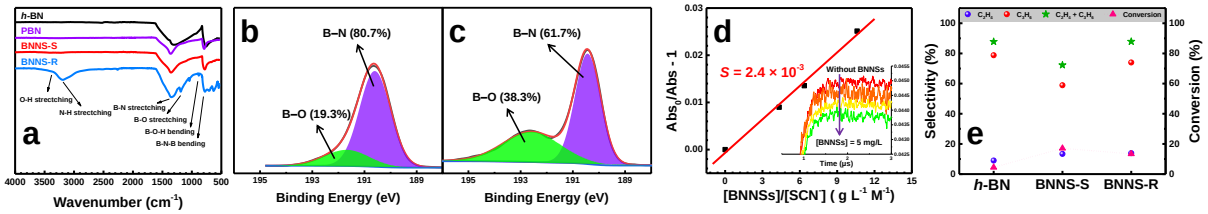

Figure 1. (**a**) ATR-FTIR spectra of different BN materials, XPS B 1s spectra of (**b**) **BNNS-S** and **BNNS-R**, (**d**) measurement of reaction rate constant using competition kinetics method, and (**e**) catalytic performance in ODHP reaction using different BN materials.

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γ-radiation induced synthesis of Ag nanoparticles using an ionomer as size regulator

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Surfactants are frequently used in colloidal synthesis of Ag nanoparticles to control particle size and other structural characteristics.[1] However, surfactants are usually difficult to completely remove from the Ag surface and they may thereby influence the material properties. For example, they will blind the active sites of the Ag catalysts.[2] Here, using a type of poly(arylene piperidinium) anion exchange ionomer PTPipQ-100[3] as a size regulator, Ag nanoparticles with controlled particle size are produced by facile γ-radiation induced synthesis as shown in Figure 1a. When the ionomer concentration increases in the reaction solution, the average particle size, and the size distribution range decrease dramatically. Since the ionomer stock solution was prepared using dimethyl sulfoxide (DMSO) as the solvent, control experiments were performed to test the effect of solely DMSO (Figure 1b). It is found that the Ag particle size is controlled by both the ionomer and DMSO. Moreover, the ionomer could be used as a stabilizer for Ag nanoparticles in colloidal suspensions. Figure 1c shows that the Ag nanoparticle is coated by a 1 nm thick layer of ionomer (amorphous layer with light color). The energy-dispersive X-ray spectroscopy (EDS) mapping (Figure 1f) of nitrogen element confirms the presence of ionomers on the surface of Ag nanoparticles. Since the ionomer is usually added to the catalyst layer of the electrode in fuel cells to enhance the OH^- exchange, Ag nanoparticles covered by ionomers can be used as a simplified model catalyst system to investigate the oxygen reduction reaction (ORR) dynamics in the fuel cells.

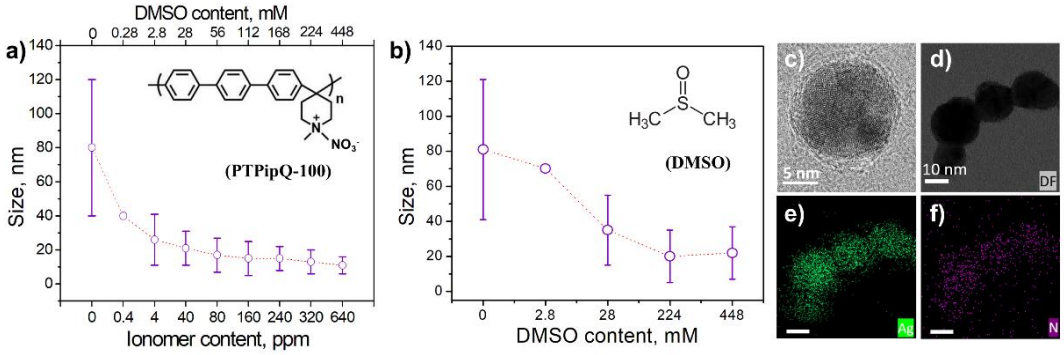

Figure 1. Ag particle size as a function of the ionomer and DMSO (a), and solely DMSO (b) concentrations in the reaction solution, error bar represents the size distribution range. High resolution transmission electron microscopy (HRTEM) image (c) and EDS mappings (e, f) of Ag nanoparticles prepared using 320 ppm of ionomer.

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POSTERS

Early, transient, highly acidic spikes in the radiolysis of water at very high dose rates: relevance for FLASH radiotherapy

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Upon being ionized into $H_2O^{\bullet+}$, water molecules dissociate rapidly (in times as short as 46±10 fs) to produce hydroxyl radicals $^{\bullet}OH$ and hydronium ions H_3O^+. It is well known that this *in situ* formation of H_3O^+ temporarily renders the spurs and tracks of the radiation more acid than the surrounding medium. This abrupt transient acidic pH effect (which we termed an "acid spike" [1]) has largely gone unnoticed in water or in living cells exposed to ionizing radiations. From a chemical and radiobiological point of view, this is rather surprising considering that many cellular processes and properties can potentially be affected by changes in pH.

While the acidic pH spikes imply low dose rates, *i.e.*, only individual, non-overlapping radiation tracks, the question arises as to whether these spikes of acidity persist even under high dose-rate irradiation conditions in which track overlap is assumed to be completed at an early point in time. If so, it would indicate the early generation of a transient acid response over the entire irradiated volume [2]. In this work, we extended our previous Monte Carlo track chemistry calculations [3] to study the influence of high dose rates on the transient yields and concentrations of H_3O^+, that are formed early during radiolysis of water by 300-MeV incident protons, which mimic the low LET (~0.3 keV/μm) of ^{60}Co γ rays or fast electrons. Figure 1 shows the evolution of the pH values over time for a few values of N (*i.e.*, the dose rate) chosen as examples between 1 (low dose-rate limit) and 2000 (~9×10^9 Gy/s) proton tracks per pulse [3]. The observed "acid-spike" effect is most intense at times less than ~10-100 ns. In this time range the pH remains nearly constant, reaching a value of ~2.8 for $N = 2000$.

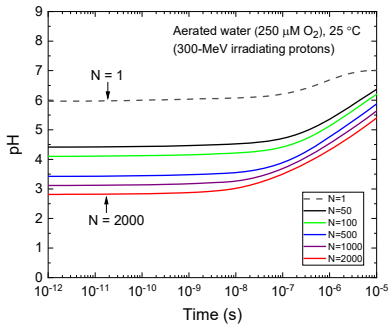

Figure 1

Given the importance of the pH value for many cellular functions, the question arises whether the generation of such spikes of acidity in cell water under high dose-rate ionizing radiation plays a role in the current radiobiological puzzle that seeks to explain the underlying mechanisms behind the FLASH effect in radiotherapy. Recall here that "FLASH radiotherapy" is a new method of irradiation in which large single doses of radiation are delivered to tumors in milliseconds. Strikingly, FLASH irradiation (intra-pulse dose rates of ~10^6-10^7 Gy/s) spares the surrounding healthy tissue while preserving the same anti-tumor activity compared to conventional-dose-rate radiotherapy (~0.03 Gy/s) that is used clinically [4].

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Contrasting reaction of hydroxyl radical with respect to ketone and thioketone group: A case study of esculetin and thioesculetin

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Radiation chemical studies of sulfur-based compounds are different from lower chalcogen i.e., oxygen. In most of the cases, the hydroxyl radical (·OH) adds to the coumarin ring or oxidises the phenolic group present in esculetin, ·OH radical reaction with esculetin produces transients that has absorption band at 410 and 510 nm. Reaction of ·OH radicals with esculetin form phenoxyl radical and OH-adducts. It is revealed that 32% of ·OH radical reaction products of esculetin are oxidising in nature whereas 47% of ·OH radical reaction products of esculetin are reducing in nature. For esculetin the ketone group is inactive towards the ·OH radical. But in the case of thioesculetin, majority of the ·OH radicals preferably react with the thioketone group. ·OH radical reactions with the thioesculetin result transients, that has absorption band at 320, 360 and 500 nm. The transient absorption band at 500 nm is concentration dependent and believe to be the dimer radical of thioesculetin. The thioketone group in thioesculetin readily react with the ·OH radical to form the dimer radical of thioesculetin. From the transients' redox nature of thioesculetin upon reaction with the ·OH radical, it is observed that 57% and 24% of the ·OH radical yielded to oxidising and reducing products respectively. The dimer radical is also characterised by quantum chemical calculations. The bond length between the two sulfur atoms in dimer radical is 2.88 Å which is less than the Van der Waals distance. Bond order between the two sulfur atoms is 0.55, suggesting that it has two center three electron (2c-3e) bond. The fate of dimer the radical of thioesculetin was established experimentally by HPLC, and it is found to disproportionate to esculetin and parent thioesculetin. Detailed reaction of the ·OH radical with its possible transient behaviour between these two compounds will be discussed.

(a) (b)

Figure 1: Chemical structure of esculetin (a) and thioesculetin (b)

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Gamma radiolysis of sunset yellow dye in aqueous solutions

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A reactive dye Synset Yellow (SY) in aqueous solutions was irradiated at doses of 0.2-5 kGy. Change of absorption spectra, colorimetric study, chemical oxygen demand (COD), total organic carbon (TOC) and pH variation were carried out and studied. It was found that the absorption band located at λ= 482 nm decreased more rapidly than the UV visible bands when irradiation dose increases. The degree of decolorization and the value of color difference (ΔE*) increases quadratically with increasing the value of radiation dose. The CODand TOC removals for the dye solutions were approximately 96% at 5 kGy. Finally, based on different spectrophotometric measurements carried out in this work showed that the kinetic degradation of synset yellow is pseudo-first order. We have also demonstrated that colorimetric study applied to a given solution could be used as a quantitative method for kinetic behaviour study.

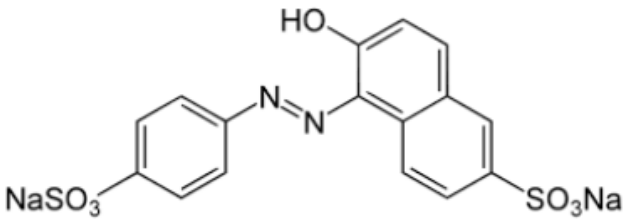

Figure 1. Chemical structure of Synset Yellow dye.

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Transformations of a Uranyl Hydroxide Phase: Probing Alteration Behavior through Humidity and Ionizing Radiation

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The fundamental chemistry of uranium minerals and their associated alteration phases is important for nuclear waste storage and the environmental mobility of uranium. Of the possible transformations at mineral surfaces, buildup of peroxide and formation of uranyl peroxides has been reported on spent fuel and depleted uranium-containing projectiles. The uranyl peroxide phase studtite, $[(UO_2)O_2(H_2O)_2](H_2O)_2$, is a secondary mineral that can form by incorporating radiation-produced peroxide at a mineral-water interface of an existing uranium-bearing mineral. Recent reports of studtite formation via alpha radiolysis are inconsistent with the existing understanding of the water-uranium-radiolysis system. Irradiating samples using an external source of radiation is therefore useful as a controlled dose can be delivered to a well-characterized specimen to study alteration products. Here we focus on the irradiation and subsequent alteration of a uranyl oxy-hydroxide hydrate phase in an effort to better probe the interfacial properties of this system.

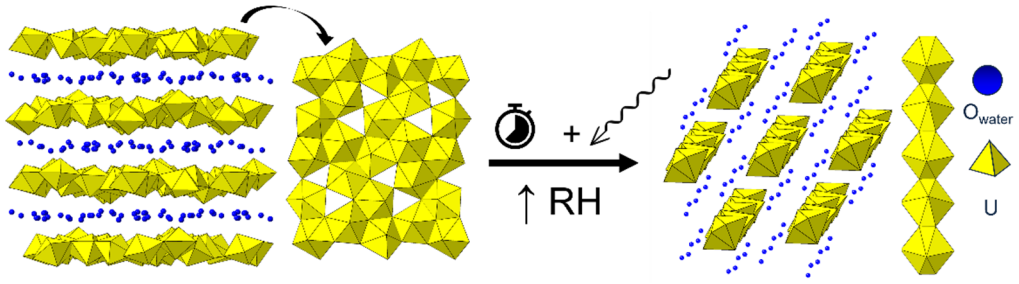

Figure 1. The transformation from uranyl hydroxide phase, metaschoepite (left) to uranyl peroxide phase, studtite (right) at high relative humidity and ionizing radiation conditions.

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Pulse Radiolysis for mechanistic studies of Ni metallaphotoredox catalysis

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The combination of photoredox and transition metal catalysis, also known as "metallaphotoredox" has enabled a host of new C–C and C–heteroatom cross-coupling reactions to be developed in recent years.[1] These reactions can be performed under mild conditions simply by illuminating the reaction mixture with light. In Ir/Ni dual photocatalytic systems, the excited Ir photocatalyst can modulate the oxidation state of the Ni catalyst by electron transfer to create reactive high energy Ni intermediates that facilitate these couplings through oxidative addition and reductive elimination steps.

Pulse radiolysis is a powerful tool to unravel mechanistic pathways in these new catalytic cycles because it enables the rapid creation of the reactive Ni species whose spectra and reactivity can be followed with transient absorption spectroscopy.

We used pulse radiolysis[2] to reduce the popular [(dtbbpy)NiBr$_2$] precatalyst (Figure 1) from Ni(II) to Ni(I). This is the first step during photocatalysis, but what happens next was not well understood. Our findings ruled out disproportionation to Ni(0)/Ni(II) or Ni(I) dimer formation as likely pathways and rates of oxidative addition of Ni(I) to a series of aryl iodides were determined.

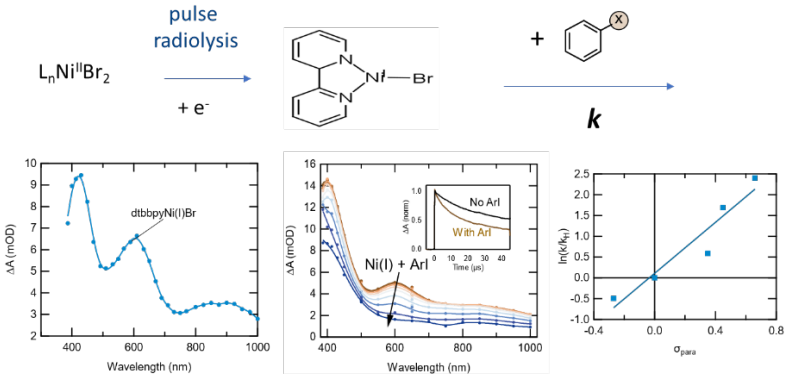

Figure 1. Generation and reactivity of Ni(I) using pulse radiolysis.

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Study on Radiolysis Mechanism of Diamide Phenanthroline Extractant and its Separation Performance for Actinides from Lanthanides

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The separation of actinides and lanthanides has been attracting increasing attention in reducing the quantity and long-term radiotoxicity of spent nuclear fuel. Diamide phenanthroline (DAPhen) extractants have been developed for group separation of actinides from lanthanides, which is important to reduce the quantity and long-term radiotoxicity of spent nuclear fuel.[1] However, the pratical extraction process suffers from strong ionizing radiation, where the degradation of solvent and extractant may degrade the extraction and separation performance for actinides.[2] Here, we evaluated the extraction performance of irradiated *N*,*N*′-diethyl-*N*,*N*′-diethyl-2,9-diamide-1,10-phenan-throline (Et-Et-DAPhen) and studied its radiolysis mechanism. The experimental results show that the distribution coefficient of U(VI) and the separation factor of U(VI)/Eu(III) dropped sharply with the increase in absorbed dose decrease sharply during EED irradiated in pure n-octanol. However, in the mixed of n-octanol and nitric acid, the distribution coefficient of U(VI) increases slightly, while the distribution coefficient of Eu(III) remains at a low level. This shows that HNO_3 can protect EED from radiolysis and some radiolysis products may have extraction properties. The possible radiolysis pathways and products of EED in the two irradiation systems are shown in Figure 1.

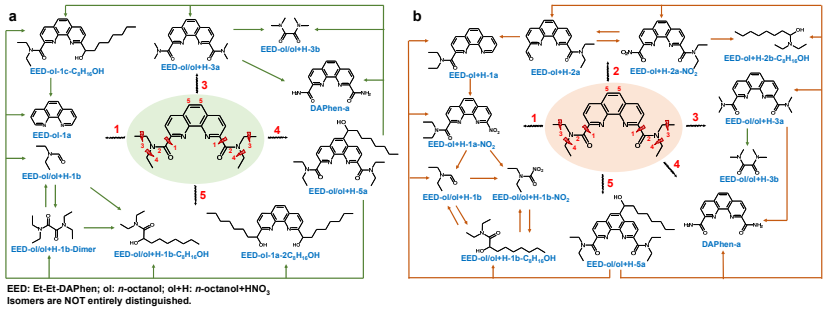

Figure 1. Proposed structure of the radiolysis pathway and products of Et-Et-DAPhen which irradiated in *n*-octanol (a) and mixture of *n*-octanol and HNO_3 (b) to absorbed dose of 400 kGy.

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Radiation Chemistry and Technology for Environment Pollution Control

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The effects of human activities in the different fields of economy have become a priority because of their environment preservation importance in the last century,. The main type of cargo transport is the sea transport, which accounts for about 90% of the volume of world trade. Consequently, global emissions from ships have increased significantly, which directly contributes to global anthropogenic emissions of SO_2, NO_x and other pollutants, and poses a serious threat to the ecosystem and public health (International Maritime Organization defined the Emission Control Area). The Institute developed and tested the Electron Beam Flue Gas Treatment laboratory system. Later on it was tested on a pilot scale for the treatment of exhaust gases from diesel engines at the Riga Shipyard, Latvia. Positive test results are the basis for designing an on-board demonstrator.

The second problem in maritime transport relates to the safety of ballast water discharges. In 2004, the International Maritime Organization developed the Convention on the Control and Management of Ship's Ballast Water and Sediments (BWM Convention). The BWM Convention entered into force worldwide on September 8, 2017. Provides a single legal regulation of ballast water management to prevent the spread of potentially harmful aquatic organisms and pathogens worldwide. The amount of harmful micro-organisms present in the discharged ballast water should be: less than 1 colony forming unit (CFU) per 100 ml of toxicogenic *Vibrio cholera*; less than 250 cfu per 100 ml of *Escherichia coli*; less than 100 cfu per 100 ml of *Intestinal Enterococci*. Laboratory tests have confirmed the feasibility of eb, and a continuous flow system design is under development for use on a floating dock. The design of the advanced wastewater irradiation room has been developed taking into account the limited space available for shielding construction, which must restrict X-ray emission.

Finally, eb is being tested for hygienization of sludge waste from municipal wastewater treatment plants. The Waste Framework Directive 2008/98/EC establishes some basic principles for waste management: it requires that waste is managed without endangering human health or harming the environment and, in particular, without risk to water, air, soil, plants or animals. The main problem related to application of this high value organic fertilizer in agriculture is contamination with human and animal parasites, their eggs, and pathogenic bacteria. According to the concept of zero-energy sludge hygienization technology, biomass from wastewater treatment plants after anaerobic digestion (electricity generation for accelerator power supply) and postferment is irradiated with electron beams.

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Radiation chemical studies of deep eutectic solvents and application as host matrix in radiation-assisted synthesis of photoluminescent tin oxide nanospheres

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Recently, DESs are being considered as cost-effective, non-toxic and biodegradable alternatives to the ILs. Hence, it is of extreme importance to study the effect of radiation and radiolytically generated transients in this media in order to appropriately use them in radiation related applications or wherever electron transfer and transport processes are involved.

Existence, yield, and properties of solvated electrons in three deep eutectic solvents, reline, ethaline, and glyceline composed of choline chloride as hydrogen bond acceptor and urea, ethylene glycol (EG) and glycerol (Gly) as hydrogen bond donors, respectively at a molar ratio of 1:2 have been experimentally studied using nanosecond pulse radiolysis (fig 1).[1] The varied transient absorption spectra of solvated electrons in these DESs have been explained on the basis of polarity, hydrogen bonding effect and the moieties responsible for creating the environment for solvation. The yield and average life time follow the trends in viscosity as well as the reactivity of electrons with the components. The C_{37} value is the highest in ethaline (with nitrate ions), indicating the slowest solvation process in this DES.

The DES, reline has been used as the host matrix and as stabilizing agent for synthesis of photoluminescent (PL) tin oxide nanoparticle.[2] Addition of any external oxido-reductive or stabilizing agent could be avoided by the use of Reline. Radiation chemical technique proved to be more appropriate in providing control over size and morphology compared to the solvothermal process. Cytotoxicity data demonstrate that the nanoparticles are suitable for application in biological studies involving cells up to a concentration of 10μM. Imaging experiments with these photoluminescent nanoparticles exhibit their ubiquitous distribution including nucleus of the tumor cells, which signifies potential application of these NPs for tagging drugs in cancer chemotherapy.

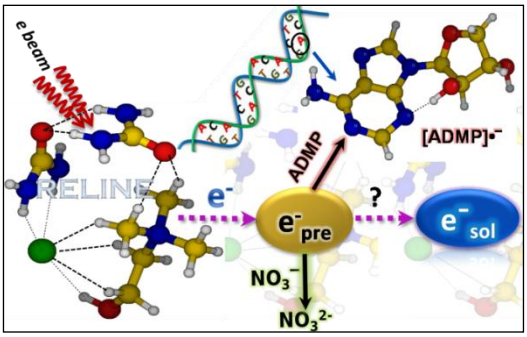

Figure 1. Schematic showing generation and reaction of pre-solvated and solvated electrons in DES

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Atomic-oxygen-induced Microstructure Formation on Polymers: Higher-order Structure Effects on Morphologies

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Atomic oxygen (AO) is a dominant constituent of residual atmosphere in low Earth orbit (LEO). Spacecraft collides with AO at a velocity of 8 km/s (5 eV). Polymers used for thermal control materials are oxidized and eroded by AO collisions, degrading their mechanical and thermo-optical properties. Thus, it is necessary to evaluate materials' durability against AO before launching. In the erosion process, AO can form nano- and microscale protrusions on a polymer surface. If the surface morphology and physical properties (e.g., wettability and optical property) can be determined by AO irradiation, it might be useful in surface modification for various polymers. However, the mechanism for the microstructure formation has not been understood yet. This study aims to understand the reason why the morphologies of AO-irradiated surfaces are different among hydrocarbon polymers with a simple chemical structure: polyethylene (PE), polypropylene (PP), and polystyrene (PS). We focused on the difference in their "higher-order structure." They have different glass transition temperature (T_g), indicating polymer chain's motion differs each other. This might affect surface scattering of AO. In addition, they have different sizes of free-volume holes, which might affect penetration depth of AO. This presentation shows (1) the temperature dependence of the morphologies and (2) the changes in free-volume holes' sizes due to AO irradiation.

PP and PS films were irradiated with AO at room temperature, 50°C, and 80°C. Their mass losses were similar regardless of polymer's type or temperature. However, the formed protrusions became larger and fewer with increasing temperature. This shows that the polymer chains' thermal motions (fluctuations of higher-order structure) affected the surface morphologies. In addition, the sizes of free-volume holes were evaluated for PE, PP, and PS by positron annihilation spectroscopy (PALS). The sizes were larger in order of PS, PP, and PE before AO irradiation. The AO irradiation decreased the free-volume holes' sizes on the surfaces. In this presentation, we will also report the correlations between polymer's type and AO penetration depth based on the PALS results.

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Radiation-assisted synthesis of photoluminescent cyclodextrin passivated Tellurium nanocomposites: Mechanistic studies and biomedical applications

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In the current work, Tellurium-based nanocomposites (Te NCs) have been prepared by using electron-beam sourced from a linear accelerator (LINAC). Te-based nanomaterials have attracted a lot of interest in recent times owing to promising applications in various areas, especially related to energy and healthcare.

Till now, the synthesis of Te-based nanomaterials has primarily been reported to be carried out using conventional wet chemical techniques, which have a number of limitations. In the present work, Te NCs were prepared in aqueous solution *in few seconds* with simultaneous passivation by a-cyclodextrin (a-CD). An important highlight of this work is the photoluminescence from the as prepared a-CD functionalized Tellurium-based nanocomposites (a-CD@Te NCs). Moreover, their size could be easily tuned by varying the absorbed dose as revealed from the UV-Vis absorption spectra and TEM studies. The formation mechanism of Te NCs was investigated by pulse radiolysis technique. The transient absorption spectra showed a peak at 360 nm, which could be assigned to the formation of Te-based intermediate species through the reaction of solvated electron with the precursor molecules. The concentration-dependent decay traces at 720 nm confirmed this observation. Further, the cytotoxicity studies of a-CD@Te NCs revealed their differential toxicity in tumor verses normal cells, with the toxic effects significantly higher in the former.

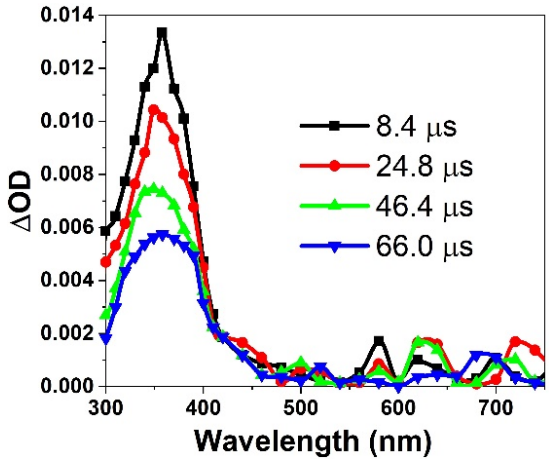

Figure 1. Transient absorption spectra of the aqueous solution of Na_2TeO_3. (2 μs pulse, ~30 Gy).

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The Study on the γ-Radiolysis of Ammonia Solution

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The radiolysis of coolant in the primary circuit occurs, producing strong oxidizing substances such as H_2O_2, O_2, and ·OH. These oxidants aggravate the stress corrosion cracking (SCC) of structural materials in the reactors. Ammonia is therefore added into the primary circuit to eliminate the oxidants in order to suppress the SCC in the VVER reactors. The present work has studied the γ-radiolysis of ammonia solution under different conditions including ammonia concentration, saturated gas, gas-liquid volume ratio, and absorbed dose. H_2O_2 is significantly inhibited with the increase of the ammonia concentration, while the concentration of NO_2^- first increases and then decreases due to the complicated redox process. Increasing O_2 promotes the formation of H_2O_2 and the consumption of NO_2^- by subsequent reactions. Whereas the H_2O_2 and NO_2^- are not detected in the systems saturated with N_2, H_2, and Ar. The increasing air volume in the closed system boost the H_2O_2 formation and the consumption of NO_2^-. The concentration of H_2O_2 increases significantly with the absorbed dose, and the NO_2^- concentration reaches the maximum (> 100 μM) when the absorbed dose is 8 kGy. This work is expected to provide a helpful reference for the optimization of the ammonia-containing coolant system.

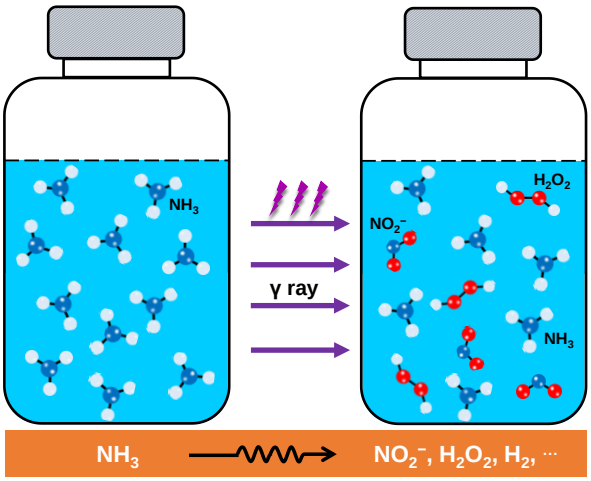

Figure 1. Schematic diagram of the production of H_2O_2 and NO_2^- by the radiolysis of ammonia solution

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Profiling DNA Damage Induced by the Irradiation of DNA with Gold Nanoparticles

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The presence of gold nanoparticles (AuNPs) greatly enhances the formation of DNA damage when exposed to therapeutic X-rays. Three types of DNA damage are assessed in irradiated DNA by enzymatic digestion coupled to liquid chromatography tandem mass spectrometry (LC-MS/MS) analysis. The major type of damage is release of the four nonmodified nucleobases, with a bias toward the release of cytosine and thymine. The second most important pathway involves the formation of several common reduction and oxidation products of DNA. Lastly, eight unique modifications of the 2-deoxyribose moiety are formed, which includes the 2′,3′- and 2′,5′-dideoxynucleosides (ddNs) of the four canonical nucleosides. The yield of ddNs decreases in the following order: ddG > ddA > ddC > ddT. From the yield and distribution of products, most of the damage is considered to arise from the generation of Auger/low-energy electrons (LEEs) and their reaction with DNA.

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Preliminary study of natural radionuclides and radiological risk assessment of a forest soil in Tunisia

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Abstract

Besides some exceptions, naturally occurring radioactive materials (NORM) are present at low concentrations in the environment. However, radionuclides may present a risk that threatens human health *via* bioaccumulation for example. This study investigated the natural radioactivity levels of a forest (FR) soil sample that was collected from the region of Bizerte in Tunisia. The sample was analyzed using gamma spectrometry and the specific activity concentration for each radionuclide was determined. The average concentrations of ^{226}Ra and ^{232}Th were 5.6 and 4.5 Bq.Kg^{-1}, respectively, which are within the reported world average. The average concentration of ^{40}K was higher than the worldwide recommended value. In terms of health analysis, five radiation health hazard parameters were calculated for the FR soil sample. The absorbed dose rate in air, the annual effective dose, the mean radium equivalent activity, the external hazard index, the internal hazard index and the lifetime cancer risk were 21.98 nGy/h, 0.026 mSv/y, 4.22 Bq.Kg^{-1}, 0.11, 0.13 and 0.09 × 10^{-3}, respectively. These values were below the minimum recommended international values. In addition, correlations among natural radioactivity levels and soil physicochemical characteristics were analyzed.

Keywords: Environment, Health hazard, Physicochemical characteristics, Radioactivity, Radionuclides.

An attempt to correlate charge distribution in hydrated assymetric hemi-bonded radical anions with their structural properties

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We have explored the effect of the nature of the counterpart in aqueous hemi-bonded $(X\text{-}SCN)^{\bullet-}$ asymmetric radical anions on their polarization by monitoring frequencies of CS and CN stretches by means of transient resonance Raman. For asymmetric analog moieties we have chosen simple halides (X = Cl, Br, and I) which show gradual change in both electron affinities and hydration energies and hence should exhibit different polarizations across X-S hemibonds.

TRRR experiments were performed using probing laser line of 415 nm near the peak absorptions of all $(X\text{-}SCN)^{\bullet-}$ species. In two of the experiments (for X^{-}=Br^{-} or I^{-}) the apparent Raman spectrum contains spectral evidence of three hemibonded intermediates present simultaneously in mutual equilibria with their precursor and successor hemibonded radical counterparts: $X_2^{\bullet-} + SCN^{-} \leftrightarrow (X\text{-}SCN)^{\bullet-} + X^{-} \leftrightarrow (SCN)_2^{\bullet-} + X^{-}$. In the case of the chloride only characteristic bands coming from the mixed contributions of $Cl_2^{\bullet-}$ and $(SCN)_2^{\bullet-}$ have been apparent suggesting that $ClSCN^{\bullet-}$ resonance Raman spectrum is almost identical to that of $(SCN)_2^{\bullet-}$. This relates to the fact that the reduced mass of the Cl-S oscillator is indeed very similar to S-S oscillator. In order to extract $(X\text{-}SCN)^{\bullet-}$ (for X=Br, I) from the composite spectrum additional experiments were performed to generate off-resonance spectra of $X_2^{\bullet-}$ and $(SCN)_2^{\bullet-}$ at 415 nm in order to subtract their contributions from the composite spectrum. Ten Stokes Raman bands of the mixed dihalide anion radicals $(X\text{-}SCN)^{\bullet-}$ (for X=Br, I) were observed in the 60-2400 cm^{-1} region and were assigned in terms of the strongly enhanced 198 and 174 cm^{-1}, weakly enhanced 719.5 and 729 cm^{-1}, and moderately enhanced 2069 and 2078 cm^{-1} fundamentals, their overtones, and combinations in $BrSCN^{\bullet-}$ and $ISCN^{\bullet-}$, respectively.

Quantum chemical calculations using a range-separated hybrid density functional (ωB97x) with flexible augmented correlation-consistent basis sets support the spectroscopic assignments of the strongest fundamental vibrations to a predominantly S-X (X = Br, I) stretching mode and the features around ~720 cm^{-1} and 2070 cm^{-1} to CS and CN symmetric stretching modes, respectively. The first-order anharmonicities of 0.8 and 0.9 cm^{-1} determined for the SX stretching mode suggest a convergence of vibrational states at energies of ~1.5 and ~1.1 eV in $BrSCN^{\bullet-}$ and $ISCN^{\bullet-}$, respectively, using the Birge-Sponer extrapolation. These values, estimated for the radical confined in solvent cage, compare well with the calculated gas-phase energies required for the radicals to dissociate into X and SCN^{-} fragments. Interestingly, CS and CN bond stretching vibrational frequencies in asymmetrical $(X\text{-}SCN)^{\bullet-}$ anion radicals are shifted a few wavenumbers down or up in comparison to the symmetrical $(SCN)_2^{\bullet-}$ molecule in $BrSCN^{\bullet-}$ or $ISCN^{\bullet-}$, respectively. Considering that $ClSCN^{\bullet-}$ seems to have vibrational frequencies almost identical to $(SCN)_2^{\bullet-}$ does not grant any systematic correlation between hemi-bond polarization in this array of molecules and vibrational frequencies of CS and CN bonds. A possible explanation of such an observation can relate to a counteracting induction and migration effects in σ and π bonds, respectively, upon charge migration across the molecule.

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Effect of gamma and neutron irradiation on properties of boron nitride/epoxy resin composites

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Abstract

Improving the radiation resistance of epoxy resin (EP) is pivotal for the reliability of equipment and the safety of facilities in the nuclear industry [1]. Hexagonal boron nitride (*h*-BN) is attractive in the preparation of radiation-resistant materials due to its good radiation stability and neutron shielding capability [2-4]. In this work, *h*-BN/EP composites with enhanced radiation resistance were fabricated by solution blending. The tensile strength and thermal properties of the composites after γ-ray and neutron irradiation were investigated. The results showed that the addition of *h*-BN improved the mechanical property and the glassy transition temperature of the resin. The presence of low-level *h*-BN was favorable to enhance the radiation resistance of EP. As for composites with the 0.05% mass percentage of *h*-BN, the absorbed dose required to decrease relative tensile strength by 50% was about 300 kGy, which was higher than that of neat EP. The intrinsic mechanism of radiation resistance was attributed to the oxygen barrier effect as investigated by XPS and EPR. Then, benefiting from the absorbing neutrons capability of boron atoms, an addition of 0.55% *h*-BN to the EP resin could reduce the neutron transmittance of the resin by 5.6%. This study demonstrates that the blending with *h*-BN can increase the radiation-resistant property of EP resin, meanwhile augmenting the neutron shielding ability.

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Development of approaches to the regeneration of rubber products using irradiation

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Irradiation of waste rubbers based on saturated rubbers is one of the most promising methods of processing polymer waste [1]. Many characteristics of the polymer change because of radiolysis [2-3].

The work is devoted to the creation of new approaches to the regeneration of rubbers based on butyl rubber by describing the destruction of intermonomeric and cross-links. At the same time, due to the course of destruction processes, it is possible to obtain materials with specified viscoelastic properties [4-5].

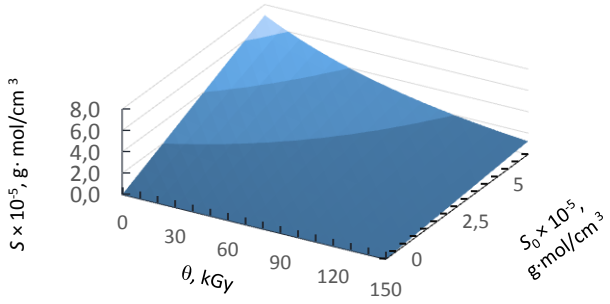

Figure 1. Dependences of the cross-linking density of irradiated rubbers on its initial value and the magnitude of the absorbed dose.

It was found that the degree of destruction of rubbers based on butyl rubber does not depend on the type of source, but is determined by the radiation dose. Within the framework of this approach, mathematical modeling was carried out. Approaches to mathematical modeling of the viscoelastic and strength properties of rubber based on butyl rubber, taking into account their multiplicative dependence on the residual crosslink density and the average molecular weight of the polymer, were first proposed.

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Development of low energy electron sources as novel chemo-radio therapeutic (CRT) agents: in-vitro study of ^{64}Cu/NOTA-terpyridine platinum in colorectal cancer cell

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Introduction: We have developed a new platinum-based complex containing terpyridine platinum (TP) compound linked to NOTA (2-[4,7-Bis(carboxymethyl)-1,4,7-triazonan-1-yl]acetic acid) as a chelator for ^{64}Cu,[2] a prolific source of low energy electrons (LEEs). We hypothesized that the LEE radiotoxicity of ^{64}Cu might synergistically interact with the chemotoxicity of the terpyridine-Pt compound within a sensitive sequence of DNA known as G-quadruplex (figure 1).[1]

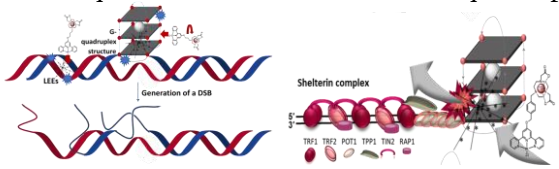


Figure 1. Proposed mechanisms of interaction between ^{64}Cu/NOTA-TP and DNA G-quadruplex.

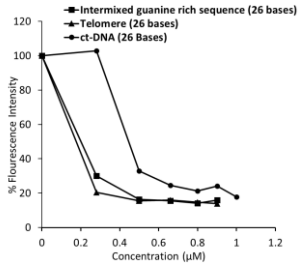
Methods: The in-vitro cytotoxicity of our ^{64}Cu-NOTA-TP complex and other control compounds were tested on colorectal cancer (HCT116) and normal human fibroblast (GM05757) cells. The affinity of ^{Nat}Cu-NOTA-TP and NOTA-TP toward two guanine-rich DNA sequences were investigated relative to a self-supplementary sequence.

Results: ^{Nat}Cu-labeled NOTA-TP complex showed 3.4, 1.7 and 2.3 times higher cytotoxicity against HCT116 cells relative to GM05757 fibroblast normal cells (Table 1, entry 2). Radiolabeling of NOTA-TP with ^{64}Cu has strikingly improved antitumor activity (EC_{50}=0.017-0.005µM), indicating a strong synergistic interaction between ^{64}Cu and platinum residue of the complex (combination index (CI)<<1, (Table 1, entry 4).

Table 1. EC_{50} values (µM) of platinum compounds for both cancer HCT116 cells and normal fibroblast.

		24h		48h		72h	
Entry	Compounds	GM05757	HCT116	GM05757	HCT116	GM05757	HCT116
1	NOTA-TPt	504 ± 4	> 700[a]	202 ± 5	63 ± 2	51 ± 3	24 ± 1[a]
2	^{Nat}Cu-NOTA-TPt	> 1000	298 ± 2	839 ± 2	481 ± 25	747 ± 26	330 ± 51
3	^{64}Cu-NOTA-TPt[b]	>200	59 ± 3	N/A	9±2	12±2	<5
4	^{64}Cu-NOTA-TPt[c]	>0.066	0.017±0.004	0.025±0.005	0.012±0.006	0.019±0.004	0.005±0.002
5	Cisplatin	88 ± 4	31 ± 2	84 ± 2	42 ± 8	77 ± 1	23 ± 3
6	Oxaliplatin	> 200	> 200	165 ± 9	64 ± 1	65 ± 3	16 ± 4

Figure 2. Guanine rich sequences affinity of ^{Nat}Cu/NOTA-TP.



Conclusion: These results highlight the potential of ^{64}Cu-NOTA-TP, which combines a radioisotopic source of LEEs with high cancer cell specificity, as a novel agent for CRT cancer treatment.

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Low-energy electron attachment to metabolites: oxaloacetic and citric acids

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In the present contribution we report results from dissociative electron attachment to molecules of biological importance, i.e. oxaloacetic acid (OAA) and citric acid (CA) [1]. Both of these acids are important metabolites found in aerobic organisms. Moreover, they contain within the molecular structure oxygen-rich functional groups which are crucial for their electron-acceptor properties that determine electron transfer processes and redox reactions during the Krebs cycle. Although the electron transfer chains established in the organism are well balanced, the delicate balance can be disturbed by the presence of "free" electrons, generated, for example, by ionizing radiation as a result of water radiolysis.

The experimental results were obtained by means of the electron-molecular crossed beam apparatus and supplemented with quantum-chemical calculations. For both OAA and CA, sharp resonance structures were observed with a maximum yield below 0.5 eV, leading to the formation of the fragment anions resulting from the decomposition of the carboxyl groups. Structures at higher energies between 3 and 9 eV were only observed for OAA, however, with much lower intensities. The results of the calculations performed indicate different mechanism, by which the near 0 eV electron is attached to the precursor molecule, leading to the formation of a negative transient ion dissociating into fragmentary ions. In the case of OAA, a transient negative ion is formed from the capture of the electron directly into some valence states, while, for the CA, dipole- or multipole-bound states mediate the transition into the valence states. It should be emphasized that both compounds while undergoing DEA reactions generate highly reactive neutral products that can lead to cell damage in a biological environment.

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Free radical reactions of atenolol and propranolol by pulse radiolysis

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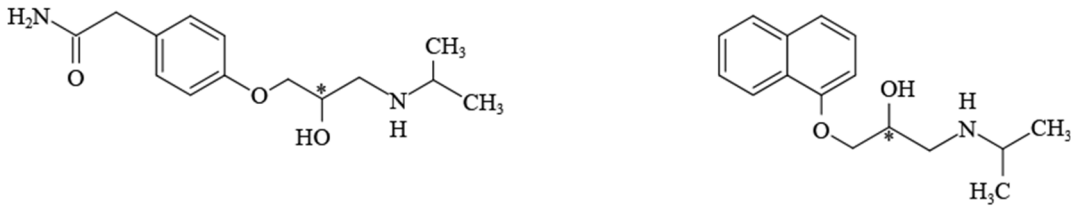
Beta-blockers, and among them atenolol and propranolol are widely applied for treatment of cardiovascular diseases. In their structure they have an aromatic ring and an oxypropanolamine side chain. They are present in the aquatic environment in ng-µg dm^{-3} concentration level [1-2]. Elimination of ß-blockers and their metabolites from the purified wastewater discharged into the environment may be implemented with low efficiency by traditional wastewater treatment technologies. Advanced Oxidation Processes are able to decompose these compounds entirely *via* formation of free radicals like hydroxyl (•OH) [3-5]. Pulse radiolysis is a suitable technique in order to get a comprehensive picture about free radical reactions.

In this study the •OH reactions of atenolol and propranolol were investigated by pulse radiolysis. In atenolol the side chain is attached to a benzene and in propranolol to a naphthalene unit (Fig. 1). •OH may attack both the aromatic parts and also the side chains. Based on their transient absorption spectra, hydroxylation on the aromatic ring (~80%) is the preferred reaction for both atenolol and propranolol. Propranolol having a condensed ring with higher electron density than atenolol showed advanced reactivity towards •OH: the rate constants of •OH reactions were 4.80×10^9 and 7.55×10^9 mol^{-1} dm^3 s^{-1}, respectively for atenolol and propranolol. The reactions of the side chain with •OH were studied by different redox titration experiments. About 10-20% of •OH may react with the side chain through formation of α-aminoalkyl and aminium type radicals in H-abstraction reaction.



Atenolol Propranolol

Figure 1. Structure of atenolol and propranolol (*: chiral carbon atom)

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Shape resonances in DNA: Very low energy electron (VLEE) induced DNA damage

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The damaging effects of ionizing radiation involve the ionization of DNA and molecules near DNA, which initially generate holes together with energetic electrons.[1] We have exposed oligonucleotides as a thin film under ultrahigh vacuum to very low energy electron (vLEEs; 1.3-2.3 eV). The formation of various types of damage as a function of dose was assessed by sensitive and highly specific LC-MS/MS analyses. The release of non-modified nucleobases (Cyt, Thy, Gua and Ade) was determined directly in DNA samples after the addition of appropriate isotopic standards. Other types of damage were determined after DNA was enzymatically digested to its corresponding nucleosides; this damage included eight products consisting of 2',3'- and 2',5'-dideoxynucleosides of the four canonical nucleosides (ddNs; ddG, ddA, ddC, ddT) and two reduction products of pyrimidine nucleosides (5,6-dihydro-5,6- dihydropyrimidines: dHT and dHU)). The release of non-modified nucleobases, in particular that of Cyt, gave the highest yield, followed by the formation of dHU, dHT and ddNs (ddG > ddA ~ ddC > ddT). In this low energy regime, we can exclude ionization as a pathway to products. The formation of all products can thus be explained by the initial formation of a transient anion (vLEEs + DNA), which decays through dissociative electron attachment (DEA) by cleavage of the N-glyosidic bond, giving rise to base release, or by cleavage of either C3'-O or C5'-O bonds of the sugar-phosphate backbone, giving rise to ddN products. In contrast, dHU and dHT likely arise from decay of the transient anion into a ground state radical anion. The yields of the above- mentioned products were found to be markedly different in long DNA strands (this study) compared to that obtained from the previously studied dinucleotide TpT.[2] This difference is explained by electron delocalization in long strands of DNA, the DEA theory of O'Malley and recent time dependent density functional theory calculations. This study broadens our understanding of DNA damage caused by ionizing radiation highlighting the damage expected to occur exclusively by the interaction of vLEEs.

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Effect of metal complexation on the DOTA radiolysis

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For both diagnostic and therapeutic purposes, radioisotopes are increasingly used in nuclear medicine. To reach the target cells in the biological environment, these elements are attached to a vector via a chelating molecule. In contact with radioisotopes, the chelating molecule is subjected to the effects of radiation, which can lead to its degradation and induce an alteration of its complexing properties. Therefore, it is important to study the impact of radiolysis on the speciation of "radioisotope-chelating molecules" complexes to identify the points of weakness of these molecules, and to guide the syntheses towards new molecules more stable in solution (or leading to less troublesome degradation products).

The ligand DOTA (1,4,7,10– tetraazacyclododecane -1,4,7,10-tetraacetic acid) has been studied for a long time because it is currently used for medical imaging, especially as a chelating molecule for gadolinium. DOTA forms very stable complexes with metals. Zirconium has a positron-emitting radionuclide, ^{89}Zr, which is an isotope of interest for medical PET imaging (Positron Emission Tomography). The complexes formed between the chelating molecules and the radioisotopes must be very stable in order to avoid the release of the metal in the body. Many clinical trials were done to find the best chelating molecule for ^{89}Zr. [1] More recently, a study showed that the DOTA ligand allowed the formation of the most stable zirconium complexes (Figure 1). [2]

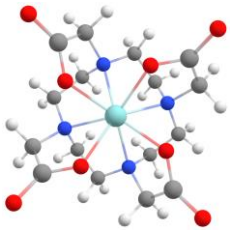

Figure 1. DFT optimized structure of Zr-DOTA complex

Previous work has been done on the degradation of the DOTA ligand under alpha irradiation. The study revealed that the ligand is degraded preferentially by decarboxylation and cleavage of an acetate arm CH_2-COOH. [3]

The aim of this study is to investigate the radiolytic stability of the DOTA ligand and the Zr-DOTA complex in aqueous solution.

In this work, the degradation products obtained by gamma irradiation were identified by Electrospray Ionization Mass Spectrometry (ESI-MS). Quantum chemistry calculations by DFT were also performed to determine binding dissociation energies (BDE) and estimate the relative strength of the bonds in the DOTA ligand free or complexed to a Zr cation.

The degradation of the ligand when complexed with Zr is significantly less important than when it is free in solution, which indicates that the metal protects the ligand from degradation. Moreover, the degradation products are different within the complex. These results have been strengthened using theoretical chemistry calculations.

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Mass spectrometric study of MeV-ion-induced reactions on submicron ethanol droplet surfaces

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The molecular-level mechanism of complicated reactions in materials induced by fast heavy ions has been studied for decades. Secondary ion emission from surfaces is a powerful probe of the reactions in heavy-ion tracks. We developed an experimental system using microdroplets to perform mass spectrometry on liquid surfaces [1,2]. In this study, we further developed a new coincidence technique between secondary ions and forward-scattered projectiles [3]. With the removal of gas-phase background signals, we revealed the various types of positive and negative ions emitted from ethanol droplets, including fragment ions, secondary reaction product ions, and cluster ions. Furthermore, the coincidence measurement provides selective information depending on the target thickness at a submicron level.

A schematic diagram of the setup is shown in Fig.1. Correlations between the time-of-flight (TOF) of positive or negative secondary ions and the energy of forward-scattered ions are recorded.

Figure 2 shows TOF spectra for positive and negative secondary ions. The production of H^+, H_3O^+, $C_2H_5^+$, and EtO^+ ions was identified as major fragment ions. These ions, except for H^+, are produced through protonated ethanol $EtOH_2^+$ after intermolecular proton transfer. The present results prove the competition between rapid hydrogen ion emission and intermolecular proton transfer accompanied by further fragmentation. Furthermore, variations in secondary ion yield, mass distribution, and kinetic energies depending on the penetration length were observed below 1 μm. These results highlight the unknown mechanism of "submicron effects" observed in secondary ion emission processes as a new phenomenon.

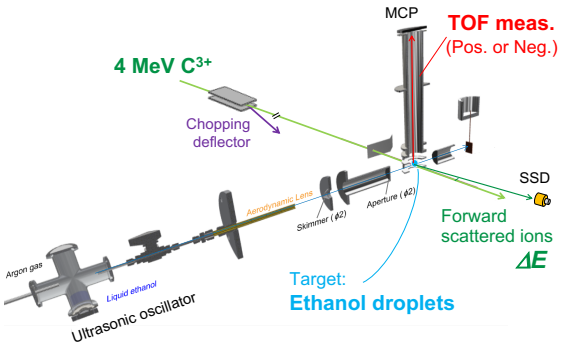

Figure 1. Schematics of the experimental setup.

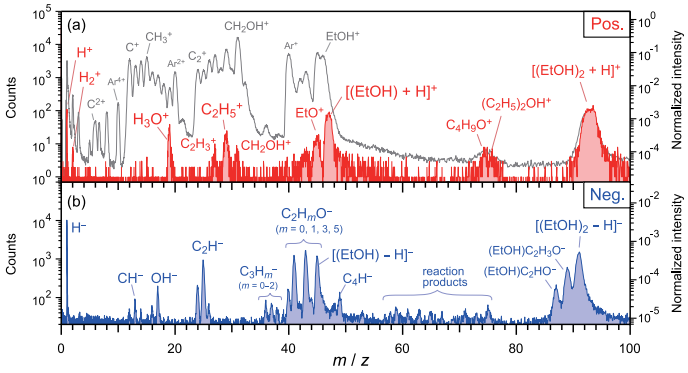

Figure 2. TOF mass spectra of (a) positive and (b) negative secondary ions from ethanol droplets [3].

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Modelling the gas generation of actinide bearing materials in storage containers (Poster abstract)

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Actinides processing generates by-products with low contents of radioactive elements. These products are placed in dedicated packaging arrangements with several containers for medium to long interim storage. However, during storage, the products evolve by generating gases as a result of radiochemical reactions. Indeed, molecules of the plastic parts of the packaging (containers, plastic envelopes), adsorbed water and matrix material of the product (salts) can be decomposed under ionizing radiation leading to the generation of primary radicals that react with others by homogeneous reactions to form stable gases [1-5].

To improve our knowledge of the evolution of these items containing alpha emitters, a model was developed using a macroscopic approach. This phenomenological model can be divided in two parts. First, plastic and water radiolysis models were used to evaluate gas generation closed to the nuclear materials. Secondly, the transportation of gases between the different containers were evaluated. The model takes into account two transfer phenomena: leakage as a result of a total pressure difference between two compartments and permeation as a result of a partial pressure gradient from each side of a plastic wall. The model was computed in Matlab using ODE solvers and was confronted to experimental measurements. Chosen key parameters were adjusted to fit the experimental data. The model allows us to highlight the parameters influencing the gas generation.

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Solvation effects on proton irradiation of DNA

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Proton irradiation of DNA is of utmost importance for many fields, from understanding radiation damage in space and Earth to medical applications for cancer treatment. Computer simulations are highly valuable tools for understanding such process, and among these, *ab initio* simulations allow us to obtain an extremely detailed description of the process down to the electronic and atomistic scale. These are, however, cumbersome due to the required level of theory, which involves simulating the non-adiabatic propagation of the electronic subsystem of the target material, and to date have been restricted to dry DNA systems, i.e., in absence of water [1], or at most with few solvating water molecules. Here we present the results of extensive ab initio simulations at the level of real-time time-dependent density functional theory, of proton irradiation of a realistic DNA system (i.e., a DNA double strand in bulk water) with pre-sampled proton trajectories [2]. We have determined different important aspects of the proton irradiation process such as the stopping power of the system, the hole/excitation distribution, the spatial distribution of the holes in terms of the depopulation of the maximally localized Wannier functions and, more importantly, the influence of the surrounding water. We show that water is neither a mere spectator on the processor nor a simplistic reducing or enhancing agent of the excitation process. Instead, water qualitatively changes the excitation landscape of the proton-irradiated DNA, making the hole population on the different atoms and bonds qualitatively different in the solvated vs. dry DNA case. These results warn against the usual practice of extrapolating results obtained in dry DNA systems to the actual DNA system in physiological conditions, and indicate that other models for estimating radiation damage in DNA may need to be revisited.

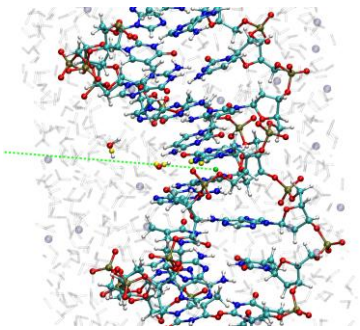

Figure 1. Solvated DNA system irradiated by a proton (green).

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How to use a MOOC in Radiation Chemistry: a toolkit for teachers

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Bring innovation in learning could be a powerful way to renovate the interest of the younger generation in disciplines not so widespread but essential for addressing current challenges of modern society. Supporting teachers by providing well designed usage models of educational materials developed on innovative learning strategies able to engage the students and facilitate their durable learning could be the breakthrough needed today/turning point in several fields.

In this perspective, an attempt has been made by developing a Massive Open Online Course (MOOC) dealing with the various applications of Nuclear Chemistry and Radiochemistry (NRC) in relevant areas of our society. The MOOC, titled "Essential Radiochemistry for Society", has been developed thanks to the support of the European MEET-CINCH project (A Modular European Education and Training Concept In Nuclear and RadioCHemistry) and is available at the Polimi Open Knowledge platform (https://www.pok.polimi.it/, Figure 1).

However, the recent pandemic situation has overwhelmingly demonstrated how such e-learning resources, developed by recognized institutions, have provided a valuable opportunity to ensure high-level training even under such constraining conditions, through the ready availability of flexible, adaptable, well-designed and securely sourced learning materials.

In the present contribution the MOOC is overall presented and its potential use in the context of radiation chemistry is discussed by proposing a specifically designed usage model. The result achieved is intended to be a MOOC usage toolkit for teachers ready to be used or an example for inspiring further MOOC usages even better tailored to the one's own needs.

Figure 1. MOOC titled "Essential Radiochemistry for Society" available at https://www.pok.polimi.it/.

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Radiotactic Colloids: towards decontamination nanorobots

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Nuclear decontamination is achieved by washing, mechanical cleaning, chemical/electrochemical treatments, etc. However, decontaminating complex geometries (ex. pipe, tank, etc.) is difficult and causes high radiation dose, more equipment, waste, contaminants release/uptake [1]. Since decades, these methods for nuclear decontamination have not developed much and stays very tedious. Therefore, a cost effective solution, withstanding high ionization radiation dose, with autonomous detectability for radiation hotspots is required to overcome the tediousness. Radiotactic colloids; Active Janus Particles (Radiotactic Nanorobots), deriving energy from Radiolysis Products; H_2, H_2O_2 could offer a possible alternative.

Janus particle is one structure system with two or more chemical discrepant composites. This asymmetry of Janus particle makes multiple synergetic functions [2] possible, therefore becoming the best candidate for the role of Radiotactic Nanobot. Active Janus Particles would derive its energy for movement from the products of radiolysis (Fig.1). Chelatants functionalized surface for radioactive material would provide decontamination abilities (Fig.2). From the available research and high stability of Gold Nanoparticle, this study focuses on the development of Gold/Silica Janus Nanoparticles, its motion study and interaction with radiolysis products on micro and macro scale.

The Gold/Silica Janus Particles have been synthesized, following Pickering emulsion strategy [3]. Firstly, modulation of the size of Silica Nanoparticles, to evaluate the gold functionalization and its mobility in H_2O_2 concentration flux will be studied. Secondly, different geometries with increasing complexity will be investigated.

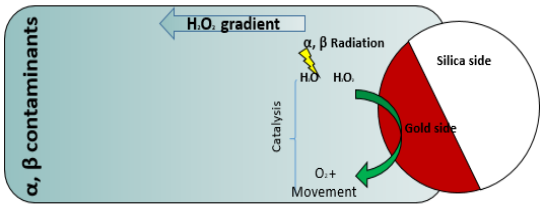

Figure 1. Movement in Gold/Silica Janus Nanoparticle (AuSNP)

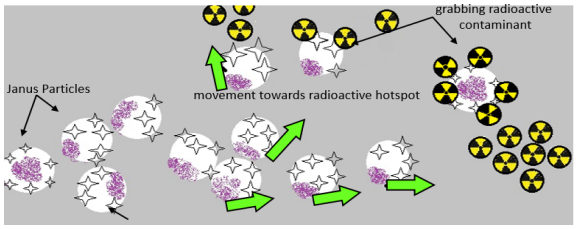

Figure 2. Radiotactic Nanobot (functionalized AuSNP) moving towards the source of radioactivity

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Au-PNiPAAm hydrogel nanocomposites as photoactuators for direct optical to mechanical energy conversion

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Recently, the one of the fastest growing areas in materials sciences is the development of polymer-based smart materials, which can autonomously change their physical and/or chemical properties under external stimuli. Photoactuators as a class of smart materials that can produce a reversible mechanical deformation under light stimuli have attracted tremendous interest due to their potential applications in soft robotics, smart grippers, artificial muscles, and smart devices. Thermosensitive hydrogels with gold nanoparticles (AuNPs) are probably the most commonly used active layers. Under the visible light irradiation, the local photo-thermal shrinking is induced, which enables the external wireless remote control of hydrogels and photo-thermal-mechanical motions such as bending, curling, and spiraling [1-3].

In this work, hydrogel nanocomposites based on thermosensitive poly(N-isopropylacrylamide) (PNiPAAm) and AuNPs were produced by radiolytic method. The presence of AuNPs, nanospheres and nanorods, incorporated into PNiPAAm hydrogel was confirmed by UV-Vis spectroscopy, XRD, TEM and SEM. The influence of different shapes of AuNPs on physicochemical properties of Au-PNiPAAm hydrogel nanocomposites was investigated. Swelling and deswelling kinetics in water at 25°C and 48°C, respectively, indicate that all samples showed non-Fickian diffusion (both diffusion and polymer chains relaxation processes control the fluid transport). On the other hand, volume phase transition temperature (VPTT), can be adjusted by the incorporation of different shapes of AuNPs. It has been observed that VPTT decreases from ≈32.5°C for Au nanorods to ≈30.5°C for Au nanospheres. Moreover, Au-PNiPAAm hydrogel nanocomposites possess an excellent "on–off" thermo-switchable electrical conductivity, especially in the case of Au nanorods.

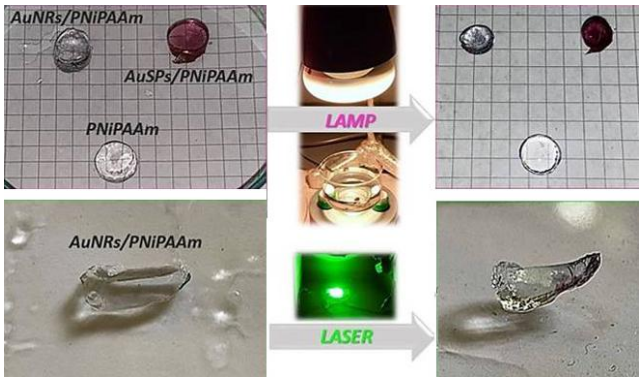

Figure 1. Photo-thermo-mechanical effects on Au-PNiPAAm hydrogel nanocomposites induced by the lamp (up) and laser (down) irradiation.

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Application methods and irradiation atmosphere for radiation crosslinked polymer nanocoatings

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Corrosion is a spontaneous degradation of a material (usually a metal) which causes a lot of financial losses in the world every year. Because all metals tend to convert into a more stable form, the process of corrosion can never be fully stopped from happening, only slowed down. Self-assembled molecular layers (SAMs) are one of the newest methods of protection that are being researched. Fatty acids have self-assembling properties with an affinity for metals and their degradation products are mostly non-toxic making such protection environment friendly compared to conventional methods. Also, SAMs are easy to prepare, cheaper and safer for people working with them. In order to prolong their longevity, and improve their stability and protective properties, SAMs are being crosslinked with ionizing radiation (gamma rays) which results in more resistant and stronger coatings.

The efficiency of protective coatings depends on many parameters, primarily depending on the preparation procedure. In this research, the influence of irradiation atmosphere and method of applying fatty acids to the surface of copper was investigated. The fatty acid used to form SAMs on the surface and for crosslinking into a protective coating was elaidic acid $C_{18}H_{34}O_2$ (EA), an unsaturated trans fatty acid. Crosslinking in air was compared to crosslinking in water and three application methods of EA from an ethanol solution onto copper were investigated: (1) immersion, (2) application by spraying and (3) application by brush.

The crosslinked coatings protective properties were investigated in simulated atmospheric conditions by electrochemical techniques, contact angle goniometry and FTIR spectroscopy. The coatings irradiated in air with 110kGy showed the best protective properties. Slightly inferior properties are seen in samples irradiated in water with 40kGy. The best method of applying SAMs of EA on copper turned out to be by immersion, followed by application with a brush and finally spraying.

Acknowledgments: We thank the Croatian Science Foundation (HRZZ IP-2020-02-4344) for supporting the research.

Preparation of oligochitosan by gamma irradiation of solution chitosan with hydrogen peroxide and survey of antioxidant activity

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Chitosan with low molecular weight and oligochitosan are attracting interest due to solubility in water and outstanding biological characteristics such as increased antioxidant capacity. This study aims to research the degradation of chitosan by gamma irradiation of mixed solution of chitosan (5 %) and H2O2 (1 %) to produce oligochitosan. The molecular weight was measured by gel permeation chromatography (GPC). The structure of oligochitosan was examined by Fourier-transform infrared (FT-IR) and ultraviolet visible (UV-vis) spectra. The results demonstrated that in the radiation dose range of 10 to 20 kGy, oligochitosan with Mw <10 kDa was effectively prepared. Using 2,2'-azino-bis (3-ethylbenzothiazoline-6-sulphonic acid) (ABTS•+), the antioxidant activity of chitosan and oligochitosan (44,4; 17,4; 10,2 and 4,1 kDa) was examined. The results revealed that low-molecular-weight oligochitosan has higher antioxidant activity than chitosan and high-molecular-weight oligochitosan. With a reaction period of 90 minutes, the antioxidant activity of chitosan and oligochitosan samples with Mw of 44,4; 17,4; 10,2 and 4,1 kDa reached 69,9; 84,5; 89,2 and 99,3 % respectively. As a result, oligochitosan prepared by gamma Co-60 irradiation has the potential to be used as a natural antioxidant.

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Pulse Radiolysis Reveals the Role of Bimetallic Interactions in Enhancement of Catalytic CO_2 Reduction by a Macrocyclic Cobalt Catalyst

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A combination of pulse radiolysis time-resolved IR spectroscopy (PR-TRIR),[1] corroborated by density functional theory (DFT) calculations and IR spectroelectrochemistry (IR-SEC), afforded characterization of all major steps of the proposed catalytic cycle for the reduction of CO_2 to CO promoted by the macrocycle, $[Co(HMD)]^{2+}$ (HMD = 5,7,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradeca-4,11-diene).[2] Bimetallic reactivity of two metal centers was identified as the primary route of catalysis. A bimetallic intermediate is formed *in-situ* from two singly-reduced $[Co(HMD)]^{+}$ species bridged by a CO_2 molecule, and the presence of a coordinating species, e.g., formate anion, appears to assist in the formation of such an intermediate. It has been demonstrated that this reactivity enables access to elementary steps with lower energy requirements, resulting in overall catalysis being kinetically more facile as compared to the mononuclear pathway. A two-step approach that combines chemical reduction followed by PR-TRIR has been successfully used for probing the structure and reactivity of reactive intermediates involved in the advanced stages of a catalytic cycle, which are rarely interrogated using experimental techniques.

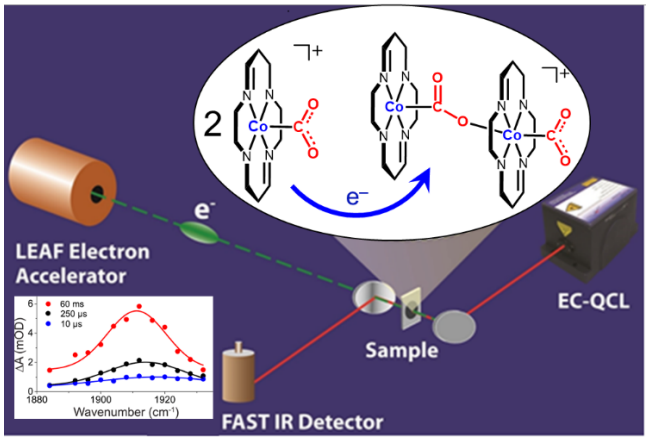

Figure 1. Schematics of PR-TRIR at BNL and key reactive intermediates in the CO_2 reduction reaction catalyzed by the $Co(HMD)^{2+}$ complex.[2]

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Fluorescence chemical dosimetry of ultrashort electron pulses

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Four different systems were investigated as liquid chemical dosimeters for low doses (< 20 Gy) with a very high dose rate picosecond-pulse electron accelerator source (~10^{12} Gy/s, ELYSE, Université Paris-Saclay). In the past, the effects of high dose rate of low-LET radiation on chemical dosimeters have been systematically studied only for the case of high peak doses (> 100 Gy) delivered by microsecond-pulse accelerators [1]. One of the systems was the ferrous sulfate (Fricke) dosimeter, but the focus of the study was on fluorescence dosimeters that offer higher sensitivity for low doses. Three established fluorescence dosimeters were selected - each utilized at a different solution pH: terephthalic acid - basic, trimesic acid - acidic, and coumarin-3-carboxylic acid (C3CA) – neutral.

The results were compared with yields determined under low dose rate radiation from a Co-60 gamma ray source (at ~10^{-3} Gy/s) – see Fig. 1. For the Fricke dosimeter, it was established that the yields were not significantly affected by the high dose rates, so it was used as a reference. Changes in the yields were not detected for the terephthalate and the trimesic acid dosimeters within the precision of the experiments; however, significant reductions of the chemical yield (- 60%) were observed for the coumarin (C3CA) dosimeter. Both the results of these investigations and the detailed discussion on the underlying kinetic reasons for these differences have been recently published [2].

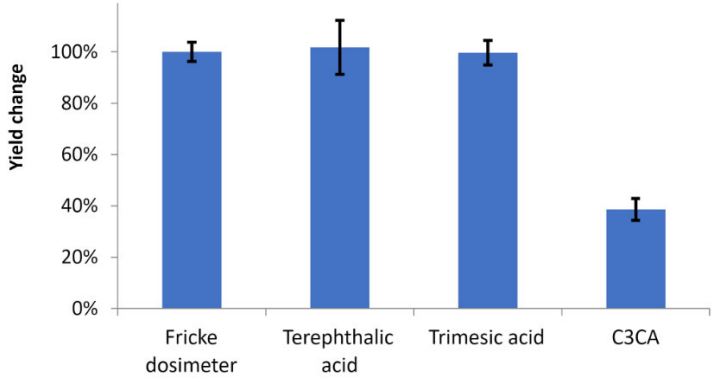

Figure 1. Change of the radiation chemical yield of chemical dosimeters caused by increasing the dose rate from 10^{-3} Gy/s to 10^{12} Gy/s for small total doses (< 10^{1} Gy) of low-LET radiation.

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A Monte Carlo Study of Nanoparticles Relevant to Nuclear Waste and Healthcare

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Nanoparticles (NPs) present in aqueous environments can cause a number of important chemical changes when subjected to irradiation. As energy is transported across the NP-water interface, and through the surrounding media, a variety of processes can occur, leading to the generation of a number of chemical species [1]. Of these produced species, molecular hydrogen (H_2), the hydroxyl radical (•OH) and low energy electrons (e^-) are hugely relevant to both the nuclear energy sector and the healthcare industry.

Along with radiation, large quantities of NP-water interfaces are present in nuclear waste storage [2]. Thus, it follows radiolytically produced H_2 can form [3]. Given the flammable and potentially explosive nature of H_2, understanding and quantifying the processes that occur within these irradiated aqueous NP environments would assist safe operations within the nuclear industry. Research is currently being conducted in the healthcare sector into the utilization of NPs during radiotherapy, as low energy electrons and •OH are known to cause damage to tumor cell DNA [4].

This presentation will show Monte Carlo (MC) simulations for a range of irradiated oxide/hydroxide NPs in aqueous environments. Novel ways of processing this data have been developed, and the resultant radial dose distributions, highlighting the processes responsible, and the positions of ionisation/excitation occurrences will be shown (figure 1).

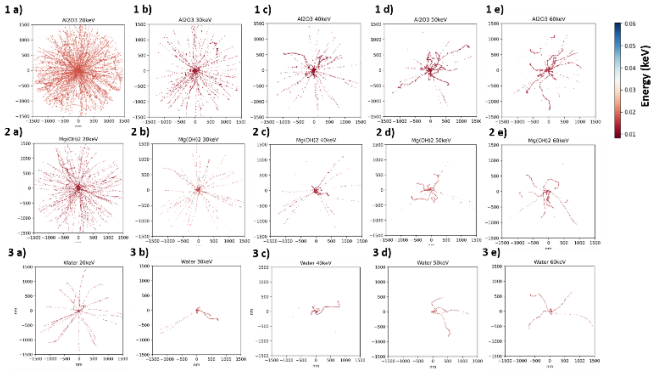

Figure 1 – An example of plots showing the position and energies of generated electrons within a 1500 nm water sphere following the irradiation of 25 nm 1) Al_2O_3, 2) $Mg(OH)_2$ and 3) water NPs by a) 20, b) 30, c) 40, d) 50 and e) 60 keV photon beams.

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Effect of ion irradiation on the work function of metals

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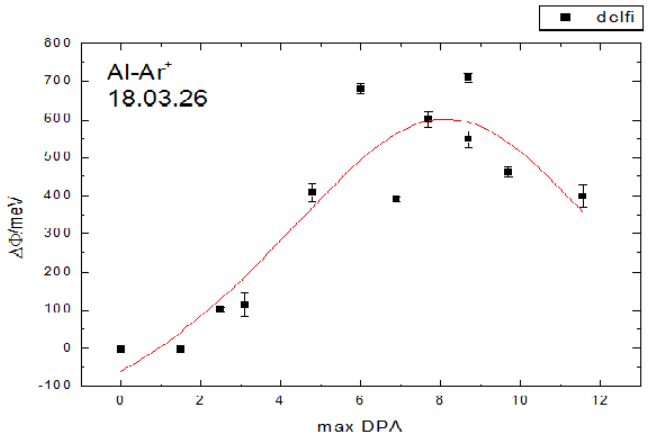
Work function is the minimum energy needed for an electron to be transferred from a metal into vacuum. Its chemical relevance includes heterogeneous catalysis, electrochemistry, and corrosion. We investigated the little studied effect of ion irradiation on work function, a process which seems to be of practical importance regarding the corrosion of nuclear reactors. A Kelvin probe equipment was used. Having irradiated crystalline iron, stainless steel, pure polycrystalline aluminium, and zinc with 40 keV H^+ and Ar^+ ions we observed maximum curves for post-irradiation work function variations as a function of particle fluence (expressed as DPA, displacement per atom). The results of Al irradiated with Ar^+ are given as an example.



We understood the observations in terms of the work function theory by considering the changes of Wigner-Seitz radii. The effect of particle bombardment on the radii, i.e. on the number densities of the metal atoms can be evaluated.

Funding Opportunities for Mobility and Radiation Chemistry Research in the EU Horizon Europe

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Horizon Europe is the EU framework programme for research and innovation. It runs from 2021 until 2027 and has a budget of €95.5 billion. It is split into different funding schemes, with three main pillars and several cross-cutting schemes. A complementary funding programme covers nuclear research and innovation.

An overview of Horizon Europe and Euroatom research and training programme will be presented. Information about various funding schemes and requirements for applying will be discussed.

Concerning the mechanism of radiation sensitization by metal oxide nanoparticles under X-ray irradiation of oxygen-free aqueous organic solutions: a spin trapping study

Ekaterina S. Shiryaeva[1], Irina A. Baranova[1], Elizaveta V. Sanochkina[1], Svetlana V. Kameneva[2], Glafira S. Taran[2], Alexander V. Belousov[3] and Vladimir I. Feldman[1]

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Radiotherapy is one of the most efficient methods of cancer treatment, and sometimes it is the only effective option. The combination of this approach with radiosensitizers was proposed to both increase the radiotherapy efficiency and reduce the unwanted effects of radiation on healthy tissues. Over the past few years nanoparticles containing elements with a high atomic number (relative to soft biological tissues) in the form of metals or metal oxide has been attracted attention as radiosensitizers. The effect of nanosensitizers is generally based on radiation physics and radiation chemistry related to the peculiarities of energy absorption and subsequent reactions of radicals in organized systems. The purpose of this work is to probe the role of different enhancement mechanisms in the X-ray irradiated oxygen-free model aqueous organic systems containing stabilized metal oxide nanoparticles.

Metal oxide nanoparticles (HfO_2, CeO_2, and WO_3) were synthesized using the approaches of sol-gel synthesis and hydrothermal synthesis. Basic features of our experimental approach for spin trapping technique with EPR detection of radiation-induces adducts with the selected spin trap (C-phenyl-N-tert-butylnitrone, PBN) were described previously [1, 2]. The main idea is that the $OH^{\bullet}$ radicals mainly produced in the system NPs/methanol/PBN/water quantitatively react with methanol to yield $CH_2OH^{\bullet}$ radicals, which form stable and easily measurable adducts $CH_2OH^{\bullet}$-PBN. The ratio between absorbed dose in the Fricke dosimeter and in the irradiated samples was determined by the Monte Carlo simulation using the Geant4 program code.

The results obtained in our study show that the sensitizing effect of metal oxide nanoparticles in the X-ray irradiated oxygen-free aqueous organic systems could be attributed to the increasing absorbed dose due to high absorption cross-section of “heavy” metal atoms known as physical enhancement. The comparison with calculations shows that using relatively small NPs probably provides the maximum value, which can be obtained for the corresponding NPs in each case (as judged by the calculations). The effects related to the so-called chemical enhancement are noticeable only for the oxygen-containing systems and were not observed in our experiments. In practical sense, these results urge the development of new efficient approaches for the radiation treatment of hypoxic media using nanoparticles.

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On the radiolytic oxygen depletion in the ultra-high (FLASH) dose-rate radiolysis of water in a cell-like environment: influence of e^-_{aq} and $^{\bullet}OH$ competing scavengers

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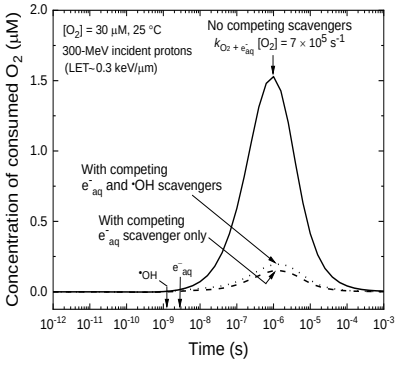
FLASH radiotherapy is a fascinating new irradiation method that uses very-high-intensity pulsed radiation (instantaneous dose rates of the order of 10^6-10^7 Gy/s) to deliver large radiation doses to tumors in milliseconds [1]. Unexpectedly, this method has been shown to minimize radiation damage to adjacent healthy tissue while preserving full anti-tumor effect when compared to conventional, much lower dose-rate (~0.03 Gy/s) radiotherapy that is used clinically. Although the exact mechanisms underlying FLASH are still unclear, it has been suggested that the high dose rates of radiation spare normal tissue *via* "radiolytic oxygen depletion" (which causes acute hypoxia and consequently temporary radioprotection). One important route proposed for O_2 consumption is based on the assumption that tissue oxygen scavenges hydrated electrons (e^-_{aq}) and $H^{\bullet}$ atoms, which are produced radiolytically from water in irradiated cells to give $O_2^{\bullet-}$ or $HO_2^{\bullet}$ depending on the pH. This hypothesis, however, has been challenged because it "overlooks the fact that reactions of $e^-_{aq}/H^{\bullet}$ with O_2, while important in the radiolysis of pure, oxygenated water, probably occur to a very small extent in cells because of the high concentrations of cellular constituents that can compete with O_2 for the capture of these species" [2]. In this work, we present some modeling data supporting the validity of this criticism.

Using our previously published Monte Carlo multi-track chemistry calculations [3], we have modeled the high dose-rate irradiation of water in a cell-like environment, *i.e.*, containing dissolved oxygen (30 μM, a concentration that is typically found in normal human cells) and scavengers of both e^-_{aq} and $^{\bullet}OH$ radicals, acting together in concert. To keep the model as bio-mimetic as possible, we used the scavenging powers for e^-_{aq} and $^{\bullet}OH$ of major cellular components previously estimated at 3.4×10^8 and 8.1×10^8 s^{-1}, respectively [4].

Figure 1 shows the evolution of the concentration of consumed O_2 over time, calculated under representative FLASH irradiation conditions (*i.e.*, ~30 Gy irradiation using 300-MeV incident protons delivered at a dose rate of 2×10^7 Gy/s [3]). In the presence of competing scavengers, the radiolytic oxygen depletion by e^-_{aq} can indeed be very small in cells or tissues, even though it is dominant in pure water [2]. Further work is needed to model O_2 depletion pathways involving reaction of O_2 with secondary radicals produced by reaction of $e^-_{aq}/H^{\bullet}/^{\bullet}OH$ with biomolecules.



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Radiation induced degradation of doxazosin

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Pharmaceuticals are widely consumed in modern societies and after use active agents and their metabolites can enter the environment via different pathways [1]. Due to high stability of pharmaceuticals in water and incomplete removal during conventional wastewater treatment processes some pharmaceuticals end up in the environment mainly in surface waters, groundwater and also in drinking water. The presence of pharmaceuticals in the aquatic environment may have adverse effects on human health which include aquatic toxicity, development of pathogenic bacteria, genotoxicity and endocrine disrupter [1, 2]. Doxazosin (DOX), a selective alpha blocker, is widely used in medical therapy as an effective antihypertensive agent. The degradation scenario of DOX under TiO_2 photocatalytic conditions, as one of the AOP processes, together with the degradation mechanism and toxicity of photoproducts have been studied recently [3].

In the present work we have focused on the degradation of doxazosin in aqueous solution by gamma irradiation. The efficiency of degradation was studied under different absorbed doses, dose rates, pH values and in the presence of radical scavengers and inorganic ions. The irradiated samples were analyzed by UV/VIS spectrophotometry and high performance liquid chromatography with diode array detector. The results indicate that •OH are the main reactive species responsible for the degradation of doxazosin, the efficiency of degradation being higher with increasing dose of gamma radiation (Figure 1.). The presence of nitrates had a stronger effect on doxazosin degradation compared to carbonates and phosphates. An optimal pH for doxazosin degradation was in the neutral, slightly acidic range (pH = 6.5), while degradation was slower under extremely acidic or alkaline conditions.

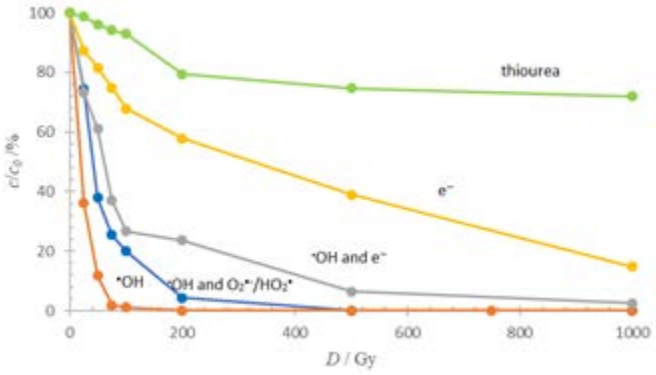

Figure 1. The influence of different radical scavengers on the degradation of DOX during gamma radiolysis.

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Microfluidic solvent extraction of cyclotron produced ^{68}Ga from zinc nitrate solutions.

Towards an automated production loop.

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The use of ^{68}Ga in nuclear medicine, specifically in cancer diagnostics, is steadily increasing. It is commonly produced by ^{68}Ge/^{68}Ga generators, but due to various drawbacks[1], e.g., the long-lived radioactive waste of ^{68}Ge, as well as increasing shortage in Ge target material and limited amounts of produced ^{68}Ga, alternative production routes of ^{68}Ga are being investigated. Especially, the production of ^{68}Ga by cyclotron irradiation of $^{68}Zn(NO_3)_2$ liquid targets is of increasing interest[2,3,4]. Current purification methods after cyclotron production consist of multi-step procedures leading to a significant loss of activity due to natural decay[2]. In this study, we describe a two-step solvent extraction process to recover ^{68}Ga from different zinc nitrate solutions by conventional batch extraction and by microfluidic solvent extraction with a liquid-liquid membrane separator, allowing for direct target solution recycling. Tested solution compositions range from 1 - 5 M $Zn(NO_3)_2$ in 0.01 - 1 M HNO_3. By using N-benzoyl-N-phenylhydroxylamine in chloroform as the extracting phase, efficiencies of up to 99.9% ± 0.9% were achieved for several different solution concentrations within 10 minutes. Recovery of ^{68}Ga from the organic solutions succeeded by back-extraction in 2 M HCl with efficiencies of up to 94.5% ± 0.6% within 1 minute. Zinc contamination in the final ^{68}Ga solution was found to be within hospital quality standards. All zinc nitrate solutions were used without any modification, possibly allowing direct recycling of the target solutions after the extraction process. Therefore, this method can potentially lead to a production loop (Fig. 1), enabling a continuous supply of ^{68}Ga.

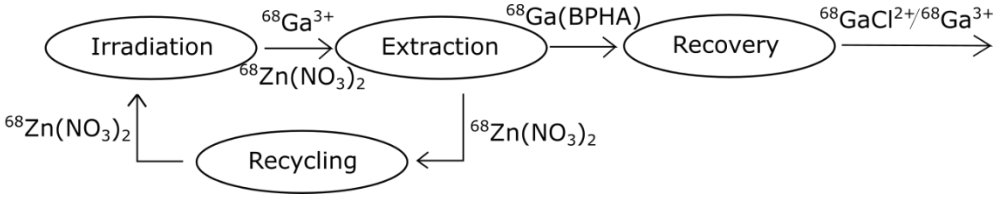

Figure 1. Irradiation and extraction loop for the continuous production of ^{68}Ga.

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Solvent-related radical ions in irradiated diethyl carbonate

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It is generally accepted that the starting point of radiation impact on organic liquids is the formation of excess electrons and solvent radical cations. According to pulse radiolysis studies of oxygen containing liquids, these primary ions may react rapidly with surrounding solvent molecules. In this study, an analysis of radiation-induced delayed fluorescence from diethyl carbonate (DEC) solutions and quantum chemical calculations were applied to examine the existence of solvent related radical cations (RCs) and anions (RAs) in irradiated DEC.

Experiments on time-resolved magnetic field effects in the recombination fluorescence (Figure 1) can be fitted on the nanosecond time scale assuming that a significant fraction, 20-40%, of primary DEC *RCs* are stabilized via formation of dimeric structure involving solvent molecule. According to quantum chemical calculations, the spin density in these dimeric structures of the solvent related RCs is predominantly localized on two anti-parallel carbonyl groups similar to ethylene carbonate [1, 2]. These radical cationic species in DEC are comparatively stable to intramolecular proton transfer from methyl groups to carbonyl group. These structures may arise due to ionization of DEC molecules in the conformation, in which both methyl groups are in unfavorable orientations for the proton transfer.

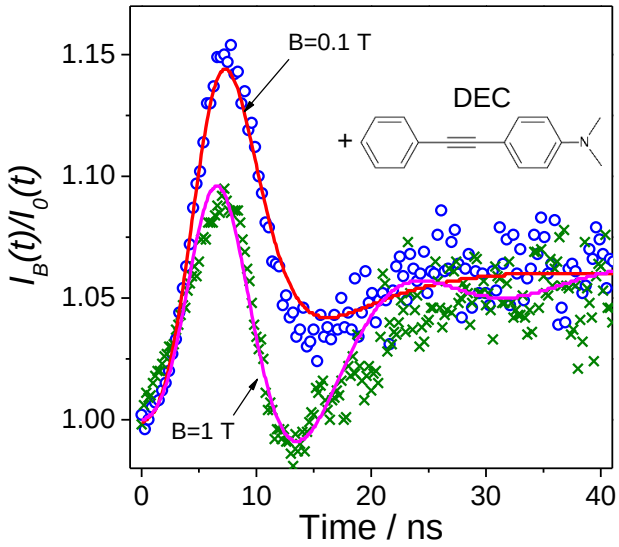

Figure 1. Experimental (o, ×) and calculated (lines) ratios, $I_B(t)/I_0(t)$, of fluorescence intensity decays at strong and zero magnetic field, respectively, for a solution of 1 mM DMAT (in the plot) in DEC at B=0.1 T or B=1 T. To simulate the ratios, two types of recombining radical ion pairs are assumed. One of the them, which results in *ca*. 20% of the observed intensity, includes a solvent related RC (and $DMAT^{-\bullet}$), while another does a solvent related RA

It looks likely that on the nanosecond timescale, excess electrons in DEC are localized on solvent molecules since the g-factor of the solvent related RA, *ca*. 2.0026, differs from 2.0023 expected for solvated electrons. Quantum chemical calculations show that such RA can be slightly stabilized by forming dimeric and trimer clusters of DEC molecules.

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The radiation-induced preparation of ultrasmall gold nanoparticles in Au(III) complexes with units of poly(1-vinyl-1,2,4-triazole) and poly(1-vinyl-1,2,4-triazole) – poly(acrylic acid)

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Unique optical, electronic and catalytic properties of gold nanoparticles (AuNPs) are the reason for the ongoing interest in AuNPs-based materials [1-3]. Ultrasmall AuNPs ranging in size from one to several nanometers are considered to be of particular interest due to quantum-size effects, their extremely high specific surface area and catalytic ability [1-3].

AuNPs with average sizes of 1.5 nm and 3 nm and narrow size distribution have been prepared in the irradiated aqueous solutions and suspensions of Au(III)-complexes with units of poly(1-vinyl-1,2,4-triazole) (PVT) and PVT – poly(acrylic acid) (PAA) respectively. The formation of AuNPs has been studied using UV-VIS spectroscopy and transmission electron microscopy. The effective stabilization of ultrasmall AuNPs is achieved due to the combination of both electrostatic interaction of polymer units and the specific adsorption of functional groups on the nanoparticle surface. The radiation-chemical approach makes it possible to obtain nanoparticles of a controlled size and containing no impurities of chemical reducing agents.

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Quantum Computing for Radiation Chemistry: Simulation of Magnetic Field Effects on Pulse Radiolysis on IBM Q

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Search for practical applications for current and near term quantum devices is critically important for the quantum computing field. Chemistry is believed to be one of the most promising fields where quantum computation offers great potential for disruption. In this work, we explore how quantum simulation of spin systems can be applied to radiation chemistry phenomena.

As a model simulation problem, we chose the time-resolved magnetic field effect (TR MFE) on recombination of radiation-generated radical-ion pairs [1]. We used the Qiskit AER quantum simulator and a real IBM Q quantum device to simulate time evolution of spin state of diphenyl sulfide$^{+\cdot}$/*para*-terphenyl-$d_{14}^{-\cdot}$ and 2,2,6,6-tetramethylpiperidine$^{+\cdot}$/ *para*-terphenyl-$d_{14}^{-\cdot}$ radical pairs. Simulated time dependencies of high-field to low-field singlet yield ratio for both radical-ion pairs are in good agreement with both theory and experimental data. More complex systems can be addressed in the future as more powerful quantum devices become available.

A novel approach leveraging the inherent qubit decoherence was used to simulate paramagnetic relaxation in the radical pairs. We have demonstrated that T_1 and T_2 qubit noise can be used to simulate paramagnetic relaxation with no additional computational overhead.

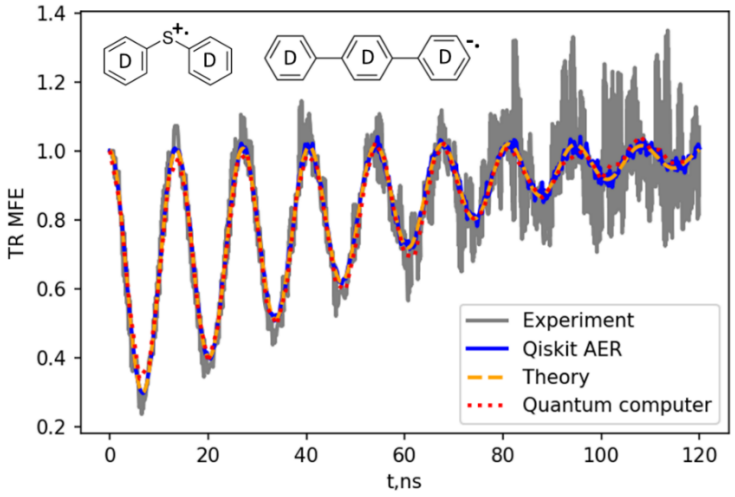

Figure 1. TR MFE simulation for the diphenyl sulfide$^{+\cdot}$/*para*-terphenyl-$d_{14}^{-\cdot}$ radical pair.

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Core-shell structured gold nanoparticles as carrier for ^{166}Dy/^{166}Ho in vivo generator

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Radionuclide therapy is a promising therapeutic modality for the treatment of cancer metastases. Radionuclides are usually bound to conventional chelators such as DOTA and conjugated to a tumor-targeting agent to selectively kill tumor cells by locally delivering ionizing radiation while sparing healthy tissue. Holmium-166 (^{166}Ho, $t_{1/2}$=26.8 h) has been recently applied in radioembolization to treat hepatocellular carcinoma or liver metastases due to its emission of high-energy beta particles. Its mother nuclide, dysprosium-166 (^{166}Dy), was found to be an alternative for the direct application of ^{166}Ho in cancer treatment. Due to the longer half-life time of ^{166}Dy ($t_{1/2}$=81.5 h), the same therapeutic effect can be achieved with less activity than ^{166}Ho, allowing for the design of an in vivo generator. However, it was reported that when ^{166}Dy was complexed to conventional chelators such as DOTA, 72% of the ^{166}Ho disassociated from the complex due to the sudden increase of charge number of ^{166}Ho ions after the internal conversion of ^{166}Dy. The highly charged ^{166}Ho ions, resulting from the internal conversion process, tend to attract electrons from surrounding atoms and thus results in the bond rupture of ^{166}Ho ions and the chelator. The free ^{166}Ho can therefore induce toxicity to healthy tissue. Thus, a carrier that can retain the internal converted ^{166}Ho has to be developed.

In this work, we incorporated ^{166}Dy in gold nanoparticles via a seed-mediated growth method. Firstly, ^{166}Dy was co-reduced with the gold precursor to form a Dy-Au nanoparticle seed. Then an extra gold layer was grown on top of the seed nanoparticles to form a core-shell structure, i.e. DyAu@Au nanoparticle. The final product had a diameter of 5 nm and a ^{166}Dy labelling efficiency of 60%. The ^{166}Ho retention tests showed that more than 95% of ^{166}Ho was retained for at least 72 hours at 37 ℃ in water. To the best of our knowledge, this is the first study to retain internal converted nuclides with gold nanoparticles. Overall, this study presents a simple, quick, and chelator-free radiolabelling method for ^{166}Dy with minimum loss of internal converted ^{166}Ho.

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Preparation of reduced graphene oxide composite aerogel by radiation method and its adsorption performance of organic pollutants

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Reduced graphene oxide (rGO) aerogel has the large specific surface area and has great application potential for decontamination of organic pollutants. In this study, γ-ray irradiation was used to irradiate the aqueous solutions containing Eu^{3+} and graphene oxide (GO), making GO self-assemble into composite aerogel under cross-linking by Eu^{3+} during the reduction process. This work explored the effects of pH, absorbed dose and Eu^{3+} concentration on composite aerogel, and studied the adsorption performance of organic dyes and organic solvents on composite aerogel. The results show that Eu^{3+} can broaden the pH range of gel formation and reduce the required absorbed dose. In addition, Eu^{3+} can effectively regulate the pore structure and reduction degree of rGO aerogel, and endow aerogel with fluorescence. The composite aerogel has excellent adsorption performance for organic solvents and organic dyes, for example the adsorption capacity of chloroform and Eriochrome Black T are as high as 386 g g^{-1} and 1300 mg g^{-1}, respectively. The fluorescence can also be used for detection and adsorption of pollutants simultaneously. This study shows that Eu^{3+} plays an important role in the synthesis of rGO composite aerogels with excellent adsorption properties.

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Transient anions in chemoradiation therapy: Enhancement of detrimental clustered lesions and crosslinks induced by 1-20 eV electrons to cisplatin-DNA complexes

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DNA is the most critical target in Radiotherapy. The molecular mechanism of platinum-based drugs in concomitant chemoradiation therapy (CRT) partly relies on enhancement of DNA damage in cancer cells, particularly that of detrimental clustered lesions and crosslinks induced by the abundant low-energy electrons (LEEs) generated by ionizing radiation.[1]

We provide the complete 1-20 eV electron-energy dependence of the yields of all LEE-induced lesions to bacterial DNA, when it binds to 5 molecules of the chemotherapeutic drug cisplatin. Damages to plasmid DNA including crosslinks, SSBs, DSBs and the loss of the supercoiled configuration were analyzed by the electrophoresis. Base damages (BDs) occurring within two turns of DNA helix were detected by the treatment of *E. coli* base excision repair endonuclease (Nth and Fpg).[2]

Under vacuum, LEEs were incident on a five-monolayer film of DNA deposited on Ta substrates. Recordings at 1-eV intervals clearly show that the enhancement of all lesions is particularly intense at the energies of core-excited transient molecular anions (i.e., TMAs at 5, 6 and 10 eV). New TMAs are observed at 14 and 18 eV, only in yield functions of cisplatin-DNA complexes. All lesions are enhanced by cisplatin, with the maximum amplification usually occuring at 14 and 18 eV. The most detrimental lesions to cell survival (i.e., crosslinks and cluster damages) exhibit highest enhancements by factors of 2-3. Whereas no cluster lesions are induced by LEEs of energy <5 eV in DNA, those of any energy cause clustered damages in the cisplatin-DNA complexes. These results confirm the current notion that LEEs and TMAs play a dominant role in the molecular mechanism of platinum-drug CRT.

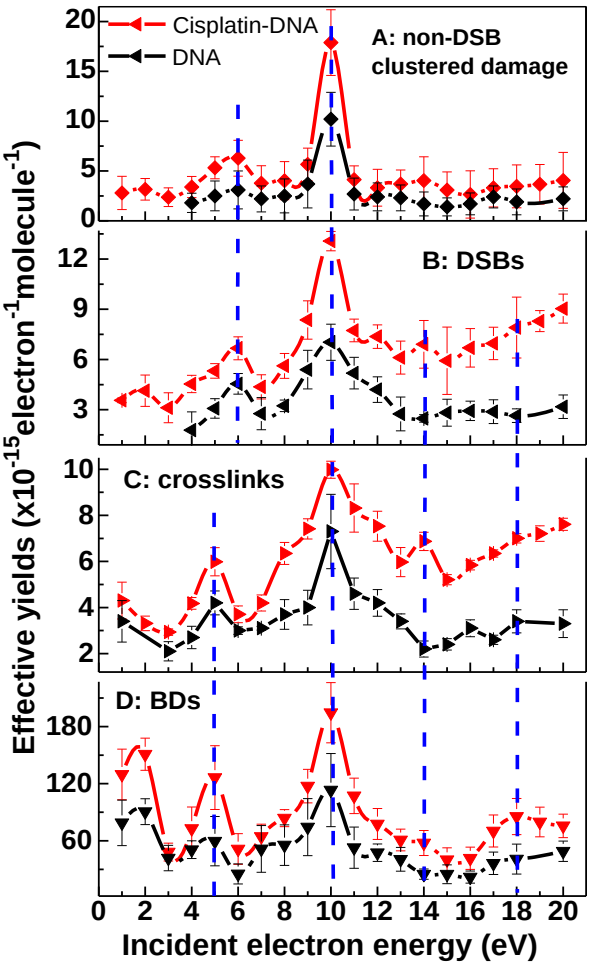

Figure 1. Yield functions of non-DSB clustered damages (♦), DSBs (◄), crosslinks (►) and BDs (▼) induced by 1–20 eV electron impact on cisplatin-DNA films of 5 ML thickness. The black points denote the yields of these lesions, produced under identical conditions, in unmodified DNA. The dash lines indicate the energies of peaks at 5, 6, 10, 14 and 18 eV.[3]

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