Polarization induced water molecule dissociation below the first-order electronic-phase transition temperature

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Hydrogen produced from the photocatalytic splitting of water is one of the reliable alternatives to replace the polluting fossil and the radioactive nuclear fuels. Here, we provide unequivocal evidence for the existence of blue- and red-shifting O–H covalent bonds within a single water molecule adsorbed on the MgO surface as a result of asymmetric displacement polarizabilities. The adsorbed H–O–H on MgO gives rise to one weaker H–O bond, while the other O–H covalent bond from the same adsorbed water molecule compensates this effect with a stronger bond. The weaker bond (nearest to the surface), the interlayer tunneling electrons and the silver substrate are shown to be the causes for the smallest dissociative activation energy on the MgO monolayer. The origin that is responsible to initiate the splitting mechanism is proven to be due to the changes in the polarizability of an adsorbed water molecule, which are further supported by the temperature-dependent static dielectric constant measurements for water below the first-order electronic-phase transition temperature.