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Verification of photo-splitting of H_2O to HOOH and H_2 as initial photoproducts

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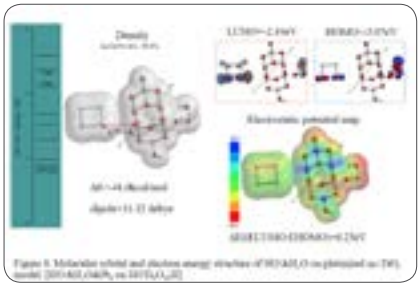
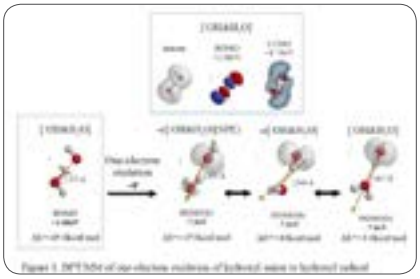
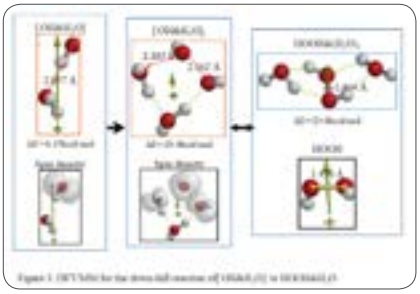
Most electrochemists and biochemists had a mindset that water oxidation yields oxygen molecules. However, Nosaka and his wife reports on generation and detection of reactive oxygen species such as HO. and HOOH in photocatalysis. We verified on the basis of density functional theory-based molecular modeling (DFT/MM) for photoelectrochemical H_2O photo-splitting systems that formation of HOOH only under photo-irradiated and highly negative bias conditions. Further literature survey revealed that, in alkali aqueous solutions (pH 8~11.5), Pt-loaded nc-TiO_2 catalyzes effective H_2O photo splitting to HOOH and H_2 as initial products. Figure 8 shows successful DFT/MM for an aggregate induced by van-der-Waals-Coulomb interactions (vdW&Clmb) between $HOTi_9O_{18}H$ as a model of nc-TiO_2 photocatalyst, HO-&H_2O as an alkali water model, and Pt_6 as platinum cluster model. Effective photoelectron transfer is verified from [HO-&H_2O] to Pt6 for production of H_2 on Pt and hydroxyl radical of [HO. & H_2O] on nc-TiO_2. Figure 1 shows DFT/MM for exothermic one-electron oxidation of alkali water model of hydrated hydroxide anion, [HO- & H_2O] to hydroxyl radical of [HO. & H_2O]. Figure 2 shows DFT/MM for exothermic vdW&Clmb- induced dimerization of the radical of [HO. & H_2O], verifying that oxidation of [HO- & H_2O] to HOOH & $(H_2O)_2$ via vdW&Clmb dimerization on nc-TiO_2. Driving force of photo splitting will be verified as due to highly exothermic electron transfer reaction to Pt_6 on nc-TiO_2.







Recent Publications

1. Wikipedia: "Photocatalytic water splitting"
2. Y Nosaka and A Y Nosaka (2017) Chem. Rev., 117:11302.
3. S Yanagida, S Yanagisawa, K Yamashita, R Jono and H Segawa (2015) Molecules 20:9732.
4. K Sayama and H Arakawa (1997) J. Chem. Soc., Faraday Trans. 93:1647.

Biography

Shozo Yanagida is an Emeritus Professor of Osaka University and a Research Director of Research Association for Technological Innovation of Organic Photovoltaics (RATO) of University of Tokyo. Since he was promoted to a Professor of newly established Koza (research course) of Graduate School of Engineering in Osaka University (1980), he had contributed to photochemical conversion of solar energy, e.g., excellent photocatalysis of both nano-sized (quantized) ZnS and poly- & oligo-paraphenylene. When he was staying at SERI (now ENREL) as a Visiting Professor of Dr. A. Nozik's group in 1984, he understood that organic molecules and their aggregates are kinds of quantum dots themselves. He has his expertise in evaluation of dye-sensitized solar cells, i.e., molecular structured photovoltaics, and enthusiasm in improving photo-conversion efficiency and long-term durability of solar cells on the basis of density-functional theory based molecular modeling.

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