9HUL¿FDWLRQ RI SKRWRFDWDO\WLF ZDWHU VSOLWWLQJ LQLWLDO SURGXFWV

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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 veri ed on the basis of density functional theory-based molecular modeling (DFT/MM) for photoelectrochemical and 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 e ective H$_2$O 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 HO$_9$Ti$_{18}$H as a model of nc-TiO$_2$ photocatalyst, HO-&H$_2$O as an alkali water model, and Pt$_6$ as platinum cluster model. E ective photoelectron transfer is veri ed from [HO$_2$&H to Pt$_6$ for production of H$_2$ on Pt and hydroxyl radical of [HO. & H$_2$O] on nc-TiO$_2$. Figure 1 shows DFT/MM for exothermic one-electron oxidation of alkali water model of hydrated hydroxide anion, [HO- &H$_2$O] to hydroxyl radical of [HO. & H$_2$O]. Figure 2 shows DFT/MM for exothermic vdW&Clmb- induced dimerization of the radical of [HO. &H$_2$O], verifying that oxidation of [HO- & H$_2$O] to HOOH & (H$_2$O)$_2$ via vdW&Clmb dimerization on nc-TiO$_2$. Driving force of photo splitting will be veri ed 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

6KR]R <DQDJLGD LV DQ (PHULWXV PHŒWLä@0L¡Š—wW W WÐLV hlhtion to Pt