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Density functional theory studies of TiO_2 for photocatalysis and Li storage applications YONG-HOON KIM, JI IL LEE, DONG KI LEE, GYU HEON LEE, JEUNG KU KANG, Korea Advanced Institute of Science and Technology — We present two theory-experiment collaboration studies of anatase TiO_2 for energy applications [1,2]. First, we discuss a hydrogen-nitrogen co-doped TiO_2 (HN-TiO_2) as a photocatalyst, and show that the interstitially introduced HN contributes to the increase of solar-to-fuel conversion efficiency. We find that the variation of valence band maximum (VBM) of NH-TiO_2 extends the photoactive spectrum to the visible light, and argue that created mid-gap states produce efficient electron and hole conduction channels. Next, we consider experimentally fabricated hierarchical TiO_2 nanocrystals integrated with binder-free porous graphene (PG) network foam [2] for a Li storage application. It was found that the TiO_2-PG facilitated rapid ionic transfer during the Li-ion insertion/extraction process. We clarify the mechanisms by showing that Li ion migration into the TiO_2-PG interface stabilize the binder-free oxide-graphene interface. Atomistic mechanism of Li ion insertion and migration is discussed by comparing cases between an isolated Li ion, when the crowding effect is included, and when the surface Li ions are present. We found that the supply of additional surface Li ions significantly reduce the Li insertion barrier, driving a spontaneous domino-like concerted Li insertion at the oxide surface region. [1] Adv. Energy Mater. **6**, 1600583 (2016). [2] Adv. Funct. Mater. **26**, 5139 (2016).

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