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Hydrogenation of Pure and Doped TiO_2 Nanoparticles for Water Splitting: Theory and Experiment

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Recently there has been an intense interest in the effect of hydrogenation of TiO_2 nanoparticles on their applications for photocatalysis and solar energy conversion through band-gap narrowing. In this work, we have carried out a quantum chemical study to elucidate the mechanism for the hydrogenation process and understand the theoretical basis of band-gap narrowing. In addition, we have investigated the effect of doping of TiO_2 nanoparticles with a small amount of transition metal atoms such as Ni, Co or Fe on the energy barriers for hydrogenation. The predicted significant reduction in the energy barriers for the hydrogenation process by doping has been corroborated experimentally. The reduction in the energy barriers for hydrogenation, from 48 kcal/mol for the pure TiO_2 to 4-9 kcal/mol for the Ni-doped TiO_2 with different dopant concentrations, for example, has significantly lowered the temperature and H_2 pressure employed. The results of theoretical and experimental studies including optical and surface characterization as well as water splitting will be reported at the conference.

Keywords: TiO_2 nanoparticles; doping; hydrogenation; water splitting; quantum chemical calculations