Band Gap Tailoring of Nd^{3+} Doped TiO_2 Nanoparticles

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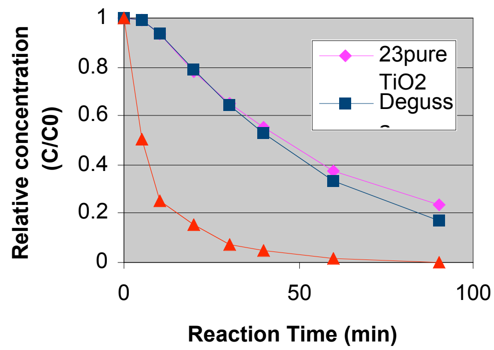
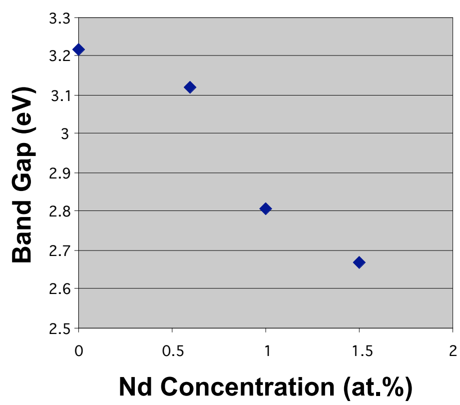
TiO_2 is a promising photocatalyst for environmental remediation processes. TiO_2 nanoparticles offer additional advantages if the size can be optimized. In bulk or large particles more than 90% of the photo-generated carriers recombine. Therefore, decreasing the total volume of the particle decreases the recombination probability making available more carriers for the oxidation or reduction of a surface adsorbed pollutant. However, there is an optimal size. Small particles have large total surface area where the surface recombination can occur. A size optimization is, therefore, required.



The large band gap of TiO_2 nanoparticles has to be tailored in order to provide additional increment in the photocatalytic efficiency. Nanoparticles, with their increased surface area, provide surface states within the bandgap to effectively reduce the band gap. However, as discussed above, the particle size cannot be decreased below a critical limit. Another way of decreasing the effective band gap is by doping with appropriate dopant. In our work, dopants such as Pt, Pd, Fe and Nd have been tried. Nd was found to be most effective in increasing the catalytic efficiency of TiO_2 of 2-chlorophenol decomposition. The enhancement is related to the relative size of the dopant and the Ti ions. When incorporated substitutionally, Nd ion being the biggest of all the dopants tested, induces stresses in the lattice which causes local charge redistribution. This, in combination with the higher electronegativity of Nd, causes oxygen vacancy formation which serves as electron traps and effectively enhance the holes lifetime. Increased hole lifetime helps in oxidative degradation of pollutants. This effect has been measured by the photocatalytic degradation of 2-chlorophenol (2-CP), as shown in Fig. 1 in which the degradation of 2-CP for various TiO_2 particles are plotted. Included in the plot is the 2-CP degradation performance of Degussa P-25 (diameter ~50nm), undoped TiO_2 nanoparticles, and Nd doped TiO_2 nanoparticles. The optical band gap of the particle is plotted in Fig.2 measured by optical absorption. This measurement has been confirmed experimentally by Near Edge X-ray Absorption Fine Structure Spectroscopy (NEXAFS) and theoretically by Linearized Augmented Plane Wave Model (LAPW).



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