Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Phonon Dispersion, Electronic Structure and Photocatalytic Properties of Rutile TiO_2 doped with X-doped (X=N, B and Pt) SANJEEV K. GUPTA, Department of Physics, Michigan Technological University, Houghton, Michigan 49931, USA, PRAFULLA K. JHA, Department of Physics, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar-364001, India, IGOR LUKAČEVIĆ, Department of Physics, University J. J. Strossmayer, Osijek, Croatia — First principles calculations were performed on the electronic, vibrational and Raman spectra of substitutional N, B and Pt-doped rutile titanium dioxide (TiO_2), within the density functional theory (DFT), using the plane-wave pseudopotential method as implemented in the ABINIT package. Of all the photocatalytic materials TiO_2 has been shown as the most useful one, with the most efficient photoactivity, the highest stability and the lowest cost. Moreover, it is safe for humans and the environment. The development of new types of photocatalytic cells is driven by the need for clean and sustainable energy. In this respect best doped materials are considered as a promising route for departing from the traditional photocatalytic cells. The physical insight provided by computational modeling may help in developing improved photocatalytic devices. To this end it is important to obtain an accurate description of the electronic structure and phonon dynamics, including the fundamental gaps and level alignment at the doped-TiO_2 interface.

Sanjeev K. Gupta
Department of Physics, Michigan Technological University,
Houghton, Michigan 49931, USA

Date submitted: 05 Nov 2012 Electronic form version 1.4