

Abstract Submitted  
for the MAR06 Meeting of  
The American Physical Society

**Electron Distributions in Pure TiO<sub>2</sub> in Anatase Phase and with Hydrogen Impurities\*** S. BYAHUT, Tribhuvan University, Kirtipur, Kathmandu, Nepal, SUDHA SRINIVAS, Central Michigan University, Mount Pleasant, LEE CHOW, University of Central Florida, Orlando, R.H. SCHEICHER, Michigan Technological University, Houghton, JUNHO JEONG, R.H. PINK, T.P. DAS\*\*, State University of New York at Albany — The electronic structures of pure TiO<sub>2</sub> in anatase phase and with hydrogen impurity have been investigated by the Hartree-Fock Cluster Procedure. They are used to study the associated <sup>47</sup>Ti and <sup>17</sup>O nuclear quadrupole coupling constants  $e^2qQ$  and asymmetry parameters  $\eta$ . For pure TiO<sub>2</sub> in the anatase phase, comparison will be made with theoretical and experimental  $e^2qQ$  in the rutile phase, the value of  $\eta$  for <sup>47</sup>Ti vanishing in the anatase phase due to local axial symmetry. \*Supported by US-Nepal Research Program, UGC Nepal, and Senior Fulbright Post-Doctoral Fellowship (S.B.) \*\*Also at UCF, Orlando

Tara P. Das  
State University at New York at Albany

Date submitted: 29 Nov 2005

Electronic form version 1.4