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First Principles Investigation of 47Ti and 17O Nuclear Quadrupole Interactions in the Rutile and Anatase Phases of TiO2[1] S. BYAHUT, Central Dept. of Physics, Tribhuvan University, Kathmandu, Nepal, SUDHA SRINIVAS, Dept of Physics, Central Michigan University, Mount Pleasant, Michigan, LEE CHOW, Dept. of Physics, Univ. of Central Florida, Orlando, JUNHO JEONG, R. H. SCHEICHER (*) , T. P. DAS (**) , Dept. of Physics, SUNY at Albany, NY — Using the First Principles Hartree-Fock Cluster procedure, electronic structures of rutile and anatase phases of TiO_2 have been investigated and utilized to calculate the nuclear quadrupole interaction (NQI) parameters for ^{47}Ti and ^{17}O in both systems. For the rutile phase, the NQI coupling constants (e^2qQ) and asymmetry parameters η are found to be in reasonable agreement with experiment for both nuclei, especially the sign of e^2qQ for ^{17}O. Experimental results are awaited for the NQI parameters in anatase to compare with our predictions, η for ^{47}Ti vanishing due to local axial symmetry. (*) Current Address: Dept. of Physics, Uppsala University, Sweden (**) Also: Dept. of Physics, University of Central Florida, Orlando, Florida.

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