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Hartree-Fock-Cluster Investigation of Nuclear Quadrupole Interactions in Solid Chalcogens, Selenium and Tellurium. M.M. ARYAL, Tribhuvan University, Nepal, N.B. MAHARJAN, Tribhuvan University Nepal, SUNY Albany, D.D. PAUDYAL, D.R. MISHRA, S.R. BYAHUT, Tribhuvan University, Nepal, R.H. SCHEICHER, Uppsala University, Sweden, S.R. BADU, SUNY Albany, J. JEONG, Univ. Ulsan South Korea, LEE CHOW, UCF Orlando, T.P. DAS, SUNY Albany, UCF Orlando — Using the first-principles Hartree-Fock Cluster Procedure, we have studied the electronic structures of pure chain like Selenium and Tellurium, pure ring structured Selenium, Tellurium impurity in chain and ring-structured Selenium and Selenium impurity in chain-structured Tellurium chain. For our investigations in all the systems we have carried out convergence studies with respect to variational basis set sizes,sizes of clusters and electron correlation effects using many-body perturbation theory. Using our calculated electronic field-gradient parameters q in the pure chain systems and employing the experimental quadrupole coupling constants (e^2qQ), the values Q(^{77}Se)=(0.50$\pm$0.04) 10^{-28} m^2 and Q(^{125}Te)=-(0.2$\pm$0.02) $10^{-28}m^2$. Results will also be presented for the asymmetry parameters η for the pure chain systems and the e^2qQ and η for ^{77}Se in selenium ring. Our calculated values for e^2qQ and η for the impurity systems will also be presented and compared with available experimental data and earlier theoretical results.

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