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Electronic Structure of Pure Selenium and Tellurium Chains and Selenium Rings and with Impurities[1] N. B. MAHARJAN, D. D. PAUDYAL, D. R. MISHRA, S. BYAHUT, Central Dept. of Physics, Tribhuvan University, Kathmandu, Nepal, HWA-SUCK CHO, Dept. of Physics, Yeung-Nam University, Taegu, S. Korea, R. H. SCHEICHER (*) , JUNHO JEONG, T. P. DAS (**) , Dept. of Physics, SUNY at Albany, NY — We have studied the electronic structures of pure chain-structured Selenium and Tellurium and with chalcogen impurities as well as ring-structured Selenium both pure and with Tellurium impurity atoms. The Hartree-Fock Cluster Theory procedure combined with many-body perturbation theory procedure has been used. The accuracy of the calculated electronic wave functions is tested by the investigation of ^{77}Se and ^{125}Te nuclear quadrupole interaction parameters. Good agreement is found with experiment for the pure systems. For the impurity systems, the agreement is reasonable but suggests the need for inclusion of more extensive relaxation around the impurity atoms. (*) Current Address: Dept. of Physics, Uppsala University, Sweden (**) Also: Dept. of Physics, University of Central Florida, Orlando, Florida

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