## Abstract Submitted for the MAR05 Meeting of The American Physical Society

Study of Binding Energies of Halogen Molecules in Solid State<sup>1</sup> M.M. ARYAL, D.R. MISHRA, D.D. PAUDYAL, S. BYAHUT, N.B. MAHAR-JAN, Central Dept. of Physics, Tribhuvan University, Kathmandu, Nepal, R.H. SCHEICHER<sup>2</sup>, JUNHO JEONG, T.P. DAS<sup>3</sup>, Dept. of Physics, SUNY at Albany, NY — As part of a program for first-principles understanding of the binding of molecules in molecular solids, we have investigated the binding energies of the halogen molecules in chlorine, bromine and iodine. For studying the electronic structures of these solid-state systems, we have employed the Hartree-Fock Cluster Procedure together with Many-Body Perturbation Theory, the latter allowing direct inclusion of Van der Waals interactions between the molecules which are found to be crucial for the stability of these molecular solids since one-electron effects in the intermolecular interactions are found to be repulsive, opposing the binding of these molecules. The VDW effect is seen to increase systematically from Cl to I, as expected form polarizability considerations.

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