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First-Principles Study of the Nature of Binding in BF_3 Molecular Solids DIP N. MAHATO, R.H. PINK, M.B. HUANG, T.P. DAS[1], SUNY Albany, ARCHANA DUBEY, LEE CHOW, UCF Orlando, MAHENDRA K. MAHANTI, NEHU, Shillong, India, R. H. SCHEICHER, MTU Houghton — The binding of BF_3 molecules in solid BF_3 is studied by the Hartree-Fock Cluster Procedure, with Van der Waals interaction between the BF_3 molecules included by the many-body perturbation theory procedure. The binding appears to be the result of strong cancellation between one-electron effects, represented by the covalent interaction between neighboring molecules combined with the coulomb interaction between the effective charges on the boron and fluorines in each of the neutral BF_3 molecules and the many-body correlation effect between electrons on neighboring molecules leading to the Van der Waals interaction, the latter being the determining factor for the binding. Quantitative results will be presented for the binding energy in this solid state system which represents a class of molecular solids for which the neutral molecular units have substantial effective charges of different signs on the constituent atoms.

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