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First Principles Study of Nature of Binding Energies in Solid Hydrogen HARI PAUDEL, University of Central Florida, SITARAM BYAHUT, Tribhuvan University, Kirtipur Kathmandu, Nepal — The study of solid hydrogen is of utmost importance since it can be used as renewal source of energy. In the present work, we have quantitatively studied the properties of solid molecular hydrogen. The Hartree-Fock method, together with electron correlation effects included by many-body perturbation theory, has been utilized in this work. Study of geometry and binding energy using different basis sets will be presented. In addition to this, the effect on energy due to orientations of hydrogen molecule at lattice point will be presented and compared with available experimental data. A comparison of binding energy using pair energy approximation and cluster energy approximation methods will be discussed.

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