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Ab-initio investigations on electronic and lattice dynamical properties on intercalation of Cu (copper) into hexagonal boron nitride(hBN). BAHADIR ALTINTAS, Abant Izzet Baysal University, Dept. of Chemistry, CIHAN PARLAK, RESUL ERYIGIT, Abant Izzet Baysal University, Dept. of Physics, CETIN BOZKURT, Abant Izzet Baysal University, Dept. of Chemistry — Layered structure of hexagonal boron nitride(hBN) and its intercalation with transition metals have been the subject of many recent studies. In this work, we investigate the electronic structure and the lattice dynamical properties of copper intercalated hBN by using Density Functional Theory(DFT) with a plane-wave basis set for the electronic wave functions and periodic boundary conditions.The interaction between valance electrons, the nuclei and the core electrons is described by norm-conserving pseudopotentials. We report the result of calculations on lattice geometry, electronic and lattice dynamical properties of the compound. Possible effects of Cu-incorporation on the structure of hBN were determined from a consideration of minimizing the quantum mechanical total energy and forces. Intercalated Cu atom is found to prefer the position between B and N atoms of two layers. The signature of intercalated Cu states were determined from the calculated electronic local density of states. The phonon frequencies were computed at the center of the Brillouin zone and four Cu-related bands were found at 187, 560, 960, 1206 cm^{-1} which can be measured by IR spectroscopy.

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