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First principles investigations into alkali intercalation of hexagonal boron nitride BAHADIR ALTINTAS, Abant Izzet Baysal University, Department of Chemistry, CIHAN PARLAK, RESUL ERYIGIT, Abant Izzet Baysal University, Department of Physics, CETIN BOZKURT, Abant Izzet Baysal University, Department of Chemistry — Although hexagonal boron nitride(hBN) is quite similar to graphite structurally, it has been very difficult to obtain any intercalation compound of hBN while there are hundreds of graphite intercalation compounds. We have investigated the possible intercalation of hBN by alkali atoms in the density functional theory framework by using pseudopotentials and plane-wave basis. The structural, electronic and lattice dynamical properties of hypothetical hBN analogues of LiC_3, LiC_6, KC_8, CsC_8, CaC_6 are calculated.We have found that although the electronic structure, band structure and fermi surface of alkali intercalated hBN is very similar to that of alkali intercalated graphite, the lattice dynamics show a set of negative frequency modes which indicate that alkali-intercalated hBN is not stable.

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