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Ab-initio study of p magnetism in CaN and CaC monolayers on Cu(001) HADI AKBARZADEH, MAEDEH ZAHEDIFAR, ZAHRA NOURBAKHSH, S. JAVAD HASHEMIFAR, Isfahan University of Technology, Isfahan, Iran — Ab-initio calculations are performed to study the p ferromagnetic CaC and CaN compounds in the zinc-blend (zb) and rock-salt (rs) structures and their monolayers on Cu(001). It is observed that within the generalized gradient functional both structures of the bulk compounds are half-metal, while the rs structure exhibits higher stability. It is argued the strong interatomic exchange interaction in these systems controls the splitting of the spin resolved bond points while it has no considerable effect on total bond strength. In contrast to the bulk compounds, the CaC and CaN monolayers on Cu(001) generally favor the zb structure and the anion terminated monolayers are more stable than the cation terminated ones. On the other hand, the anion terminated systems are non- or weak magnetic systems while the less stable cation terminated layers exhibit strong magnetization. In the case of CaN monolayer on Cu(001), the nudged elastic band calculations show an activation barrier of 1.18 eV per CaN unit between the higher energy ferromagnetic and the stable nonmagnetic terminations. Therefore, epitaxial growth of a Ca terminated CaN thin film on Cu (001) is likely a practical way to form a novel half-metal/metal junction.

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