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ADSORPTION OF ALKALI, ALKALINE-EARTH AND TRANSITION METALS ON ZR2C STRUCTURE

This study describes the structural and electronic properties of alkali (Li, Na and K), alkaline earth (Be, Mg and Ca) and transition (Cu, Ag and Au) metal adsorption on ZR2C structure. First-principles calculations based on the Density Functional Theory (DFT) were performed, using the SIESTA code with the generalized gradient approximations (GGA). The structure was generated parallel to the (1 1 1) crystallographic plane. The metals were adsorbed on the Zr atom (top T site), on the C atom (down D site), on the bond between C and Pb (bridge Ba and Bb sites) and above the hexagonal figure formed (hollow H site) of ZR2C. The transition, Na and Ca atoms are adsorbed preferentially on the H site; while Li, Be and Mg are adsorbed at the D site; and K atom is adsorbed at the T site. The results indicate that the adsorption of transition and Be atoms could have applications in storage of hydrogen, whereas Li and Na atoms for ion batteries.

Keywords

DFT, Zr2C, adsorption

Reference

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