



**titre:**

**First-principles calculations of adhesion,  
bonding and magnetism of the Fe/HfC interface**

**abstract**

First-principles plane-wave pseudopotential calculations of the adhesion, bonding and magnetism of the interface between the ferromagnetic bcc Fe and non-magnetic HfC are performed. The work of adhesion for C- and Hf-site Fe/HfC interfaces is calculated. High adhesion at C-site interface is found and Fe-C polar covalent bonds are formed across the interface. The magnetic moments of Fe atoms at interface are increased in both interfaces. The effect of the magnetism on the electronic structure of Fe/HfC interface is also investigated. It is shown that the change in band of majority-spin leads to enhance the magnetic moment of Fe.

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