

Abstract Submitted
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Comparative Density Functional study of Ti on CuN/Cu(100)¹

JESUS CRUZ, Georgetown University, PUSHPA RAGHANI, Stanford University, BARBARA JONES, IBM Almaden Research Lab — We have performed a Density Functional Theory (DFT) calculation using the Projector Augmented Wave (PAW) technique to study the electronic structure of adatoms of Ti placed on a single layer of copper nitride (CuN) surface grown on top of Cu(100). The insulating CuN surface mediates superexchange interactions between the magnetic adatoms, and also can strongly affect electronic properties. The PAW technique allows us to have elements of the precision of an all-electron (AE) calculation and the performance of an Ultrasoft Pseudopotential (USPPs) calculation. We compare results obtained of the magnetic moment, atomic positions, and charge densities of Ti adatoms with both USPPs and PAW methods, and discuss the similarities and differences between the methods. We also report studies of the effect of the Coulombic repulsion U in the PAW methodology, and compare some of these results to an all-electron calculation.

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