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Spin and exchange coupling in Ti atom and Ti dimers PUSHPA RAGHANI, Center for Probing the Nanoscale, Stanford University, Stanford, CA, USA, JESUS CRUZ, Georgetown University, Washington, D.C., USA, BARBARA JONES, IBM Almaden Research Center, San Jose, CA, USA — It is very important to know the spins on magnetic atoms embedded in a molecular network. Single or multiple magnetic atoms with a large spin can be used as molecular magnets for magnetic storage devices. We use denisty functional theory (DFT) with pseudopotentials and GGA+U to calculate spin on Ti atoms adsorbed on CuN/Cu(100) surface; and compare this spin with that obtained from scanning tunneling microscopy experiments. Then we calculate the exchange coupling for a complete layer of Ti, as well as dimers of Ti on the same CuN/Cu(100) surface.

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