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Magnetic Interaction between Surface Engineered Rare-earth Atomic Spins BARBARA JONES, IBM Almaden Research Center, San Jose, CA, CHIUNG-YUAN LIN, National Chaio Tung University, Taiwan — We report an ab initio study of rare-earth adatoms (Gd) on a surface, where it has been demonstrated previously that the STM can build and manipulate spin-coupled transition-metal atoms on such a surface one atom at a time, and have their spin excitation measured to be antiferromagnetic. The present work is the first attempt of studying rare-earth spin-coupled adatoms, the geometry effect of spin coupling, and the underlying mechanism of ferromagnetic coupling. The exchange coupling between Gd atoms on the surface is calculated to be antiferromagnetic in one geometry and ferromagnetic in another, by considering their collinear spins and using the PBE+U exchange correlation. We also find the Gd dimer in these two geometries is similar to nearest-neighbor and next-nearest-neighbor Gd atom pairs in GdN bulk. We analyze how much direct exchange, superexchange, and RKKY interactions contribute to the exchange coupling for the ferromagnetic arrangement by additional first-principles calculations of alternative model systems. Our calculations also show that the Gd spin of these structures is 7/2, the same as that of a GdN bulk.

Barbara Jones
IBM Almaden Research Center, San Jose, CA

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