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First-principles Calculation of Magnetic Anisotropy of a Single Atom on a Surface[1] CHIUNG-YUAN LIN, National Chiao Tung University, BARBARA JONES, IBM Almaden Research Center — Recent progress on scanning tunneling microscopy has made it possible to position (in atomic-scale accuracy) and probe single magnetic atom on material surfaces. Targeting the fabrication of a single-atom data storage bit, we perform first-principles calculations of single magnetic atoms (Fe and Mn) on a surface. Structure relaxation determines the binding structures of the magnetic atoms to its surroundings. Charge analysis indicates that the magnetic atoms form polar covalent bonds with the surface. Spin density is found to spread up to 4Å from the magnetic atom, which is qualitatively similar to that reported in DFT calculations of molecular magnets. Total energies with spin-orbit interaction included are calculated in different spin orientations, and are compared to the anisotropy axes measured in the experiments.

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