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Single-atom Magnetic Anisotropy on a Surface CHIUNG-YUAN LIN, JING-NENG YAO, Department of Electronics Engineering, National Chiao Tung University — Studying single-atom magnetic anisotropy on surfaces enables the exploration of the smallest magnetic storage bit that can be built. In this work, magnetic anisotropy of a single rare-earth atom on a surface is studied for the first time, both computationally and theoretically. The substrate surface is chosen to be a copper-nitrite surface, where single transition-metal magnetic atoms on the same surface were previously studied one atom at a time by STM.[1] We propose unconventional f and d subshell symmetries so that following first-principles calculations, simple pictorial analyses of such anisotropy can be performed for the first time, independently for both rare-earth and transition-metal adatoms. The analyses explain the spin-density distribution of a single adatom, and derive the spin orientation of its largest spin-orbit coupling. The magnetic anisotropy energy of the present study is calculated to be a factor of five larger than the previous highest one.

[1]C. F. Hirjibehedin, C.-Y. Lin, A. F. Otte, M. Ternes, C. P. Lutz, B. A. Jones, A. J. Heinrich, Science 317, 1199 (2007).

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