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Giant magnetic anisotropy of Co, Ru, and Os adatoms on MgO (001) surface. HONGBO WANG, XUEDONG OU, FENGREN FAN, ZHENGWEI LI, HUA WU, Fudan Univ — Large magnetic anisotropy energy (MAE) is desirable and critical for nanoscale magnetic devices. Here, using ligand-field level diagrams and density functional calculations, we well explain the very recent discovery [I. G. Rau et al., Science 344, 988 (2014)] that individual Co adatom on MgO (001) surface has a large MAE of more than 60 meV. More importantly, we predict that a giant MAE up to 110 meV could be realized for Ru adatoms on MgO (001), and even more for the Os adatoms (208 meV). This is a joint effect of the special ligand field, orbital multiplet, and significant spin-orbit interaction, in the intermediate-spin state of the Ru or Os adatoms on top of the surface oxygens. The giant MAE could provide a route to atomic scale memory.

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