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magneto-crystalline anisotropies in transition-metal Giant monowires YURIY MOKROUSOV, STEFAN HIENZE, Hamburg University, Germany, GUSTAV BIHLMAYER, STEFAN BLUGEL, Research Center Juelich, Germany — The magneto-crystalline anisotropy energy (MAE) proved to be crucial for stability of magnetism in low-dimensional structures against thermal fluctuations. Here, we report on magnetic properties of free standing 3d, 4d, and 5d transitionmetal (TM) monowires, paying special attention to the influence of spin-orbit interaction, revealing its utter importance for magnetism in these structures. The calculations were performed with the one-dimensional (1D) version of the full-potential linearized augmented plane-wave (FLAPW) method. The new 1D-FLAPW scheme [1] is extremely fast and allows a natural treatment of structures with 1D geometry. We present equilibrium interatomic distances, spin- and orbital moments, and the values of MAE. Across the series the easy axis of magnetization oscillates between two possible directions: perpendicular and along the wire axis. The largest values of the MAE occur at the end of the series. Giant values of 30-100 meV/atom can be obtained upon stretching of 4d- and 5d-TM wires. Certain chains change the magnetization direction upon wire stretching, opening new perspectives in controlling the spin-dependent ballistic conductance in these structures [2]. [1] Y.Mokrousov et al., Phys. Rev. B 72, 045402 (2005), [2] Y.Mokrousov et al., Phys. Rev. Lett. 96, 147201 (2006)

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