# Magnetic properties of 3d, 4d, and 5d transition-metal atomic monolayers in Fe/TM/Fe sandwiches: Systematic first-principles study

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Previous studies have accurately determined the effect of transition metal point defects on the properties of bcc iron [1-2] and the magnetic properties of transition metal monolayers on the iron surface have been studied equally intensively. In this work, we investigated the magnetic properties of the $3d$, $4d$, and $5d$ transition-metal (TM) atomic monolayers in Fe/TM/Fe sandwiches using the FPLO (full-potential local-orbital) scheme of density functional theory [3]. We prepared models of Fe/TM/Fe structures using the supercell method [4]. We selected the thickness of the layer such that the atomic Fe layers furthest from the TM layer exhibit the properties of bulk iron-bcc. Perpendicular to the plane of the layer, we observe charge and spin density waves in iron-bcc. We determined the values and orientation of the magnetic moments in the TM atomic layers. Furthermore, we investigate the dependence of those layers on a magnetocrystalline anisotropy energy.

**References:**

[1] H. Akai, Hyperfine Interact. 43 (1988) 253–270.
[2] P.H. Dederichs, R. Zeller, H. Akai, H. Ebert, J. Magn. Magn. Mater. 100 (1991) 241–260.
[3] K. Koepernik, H. Eschrig, Phys. Rev. B. 59 (1999) 1743.
[4] A. Edström, Phys. Rev. B 96 (2017) 064422.

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