

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Understanding surface energies of transition metals with density-functional theory ALOYSIUS SOON, MARTIN FUCHS, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG — Determining index-specific surface energies of metals is, to date, still a non-trivial task, both experimentally and theoretically. Density-functional theory (DFT) calculations within the local-density approximation (LDA) for exchange-correlation (XC) have provided understanding of qualitative trends. Yet, absolute surface energies, in particular of *d*-metals still exhibit significant uncertainties related to the description of XC: gradient-corrected functionals (GGA) which improve over the LDA for other properties often predict less accurate surface energies. This calls for a careful analysis of XC effects on surface energies, including non-local exchange and/or correlation. Here we analyze the surface energies of 4*d*-metals with modern GGA functionals (PBEsol, AM05, developed to better describe bulk solids and (jellium) surfaces than the LDA and previous GGAs), using the all-electron FHI-aims code [1]. Relating the bulk cohesive energy and surface energy via a bond-cutting model we find modern GGAs can indeed correct the poorer results of the usual PBE-GGA but worsen the bulk cohesive energies of 4*d*-metals. In addition, we consider hybrid XC functionals, using a cluster correction scheme [2], and discuss the effects of including exact exchange on the calculated surface energies.

[1] <http://www.fhi-berlin.mpg.de/aims/>;

[2] Q.-M. Hu *et al.*, Phys. Rev. Lett. **98**, 176103 (2007); **99**, 169903(E).

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Date submitted: 13 Nov 2008

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