

Abstract Submitted
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Strength of the effective Coulomb interaction at metal and insulator surfaces ERSOY SASIOGLU, CHRISTOPH FRIEDRICH, STEFAN BLÜGEL, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — The effective on-site Coulomb interaction (Hubbard U) between localized electrons at surfaces of solids is expected to be enhanced due to the reduced coordination number and the subsequent reduced screening. By means of first-principles calculations in conjunction with the constrained random-phase approximation [1] within the FLAPW method, we show that this is indeed the case for simple metals and insulators but not necessarily for transition metals and insulators that exhibit pronounced surface states [2]. In the latter case, the screening contribution from surface states as well as the influence of the band narrowing can increase the electron polarization to such an extent that the expected decrease is overcompensated. In some cases the U parameter is substantially reduced, e.g. by around 30% for the Cr(100) surface, contrary to conventional wisdom. It also depends on the properties of the surface states for different surface orientations, e.g. 10% [2%] reduction [enhancement] of U for MgO (110) [MgO (100)]. We show a systematic study for prototype materials including transition-metal surfaces.

[1] E. Şaşıoğlu et al., Phys. Rev. B 83, 121101(R) (2011).

[2] E. Şaşıoğlu et al., Phys. Rev. Lett. 109, 146401 (2012).

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