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Magnetic nature and hyperfine interactions of transition metal atoms adsorbed on ultrathin insulating films: a challenge for DFT.

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SUPPORTING INFORMATION

Table S1. Lattice parameters of MgO and Ag, strain released on the MgO film, Ag(100) work function, change in the work function in $(MgO)_{ML}$/Ag and $(MgO)_{BL}$/Ag, with respect to Ag(100), interlayer distance in $(MgO)_{ML}$/Ag and $(MgO)_{BL}$/Ag.

	a (MgO) (Å)	a (Ag) (Å)	Strain %	ϕ (Ag) (eV)	$\Delta\phi$ (ML) (eV)	$\Delta\phi$ (BL) (eV)	R_I (ML) (Å)	R_I (BL) (Å)
PBE+D2'[1]	4.253	4.162	-2.2	4.24	-0.95	-1.33	2.51	2.57
PBE+D3	4.204	4.065	-3.3	4.16	-0.98	-1.38	2.55	2.57
HSE06+D3[a]	--	--	--	3.83	-1.15	-1.27	--	--
HSE06+D3[b]	4.154	4.053	-2.2	3.89				
Exp	4.211	4.079	-3.1	4.22	-0.5/ -1.2[c]			

[a] Single point with HSE06 at the PBE+D3 geometry [b] Full relaxation with HSE06+D3

[c] Values in the range -0.5 eV/-1.2 eV are reported depending on the adopted technique (contact potential measurement vs. field emission resonance)[2]

References

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