Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Density Functional Theory studies of metal supported thin Zirconia films WERNFRIED MAYR-SCHMOELZER, FLORIAN MITTENDORFER, JOSEF REDINGER, Vienna Univ of Technology — We present the results of DFT calculations of the interface between a single layer thin ZrO_2 film and the supporting metals Pt_3Zr [1] and Pd_3Zr [2]. Both are very stable and are present when thin ZrO_2 films are grown by oxidation. Using the Vienna Ab-initio Simulation Package (VASP) employing standard PBE and van-der-Waals density functionals a thorough investigation of the structural properties was done for both small model cells and the large experimentally found super cells. Both substrates have a similar crystal structure but the binding mechanism differs: the Pt_3Zr substrate shows a pure Pt surface layer, leading to weak bonding between the film and the substrate with large nonlocal contributions. The Pd_3Zr substrate is stoichiometric and a Zr-O bond forms between substrate and oxide film, leading to higher adsorption energies. The large buckling found experimentally could be attributed to the closer distance resulting from nonlocal contributions for the Pt_3Zr substrate and to the Zr-O bond for the Pd_3Zr substrate. Furthermore we present results on the adsorption of atomic hydrogen and water molecules on the surface generated by the thin Zirconia film.

[1] Antlanger, M. et al, Phys Rev B 86, 035451 (2012).
[2] Choi, J et al, submitted.

Wernfried Mayr-Schmölzer
Vienna Univ of Technology

Date submitted: 14 Nov 2013 Electronic form version 1.4