Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Tuning surface reactivity by finite size effects: role of orbital symmetry in the $d-$band model[1] PAUL SNIJDERS, XIANGSHI YIN, VALENTINO COOPER, Oak Ridge National Laboratory, HANNO WEITERING, University of Tennessee, Knoxville — Catalytic activity depends sensitively on the strength of the interactions between reactant molecules and catalyst surface: too weak and the catalyst cannot capture enough molecules to react; too strong and the reaction products do not desorb, blocking further reactions. The ability to control the binding strength of molecules to metal surfaces is thus fundamental to the design of efficient and selective catalysts. Catalyst design often relies on increasing the interaction strength on relatively non-reactive materials by introducing active sites. Here, we present a complementary approach: we exploit finite size effects in the electronic structure of ultrathin Pd(111) films grown on Ru(0001) to tune their reactivity by changing the film thickness one atom layer at a time. While bulk Pd(111) is reactive toward oxygen, we find that Pd films thinner than 6 atom layers are surprisingly inert to oxidation. This observation can be explained with the d-band model only when it is applied to the orbitals directly involved in the bonding. The insight into orbital specific contributions to surface reactivity could be useful in the design of catalysts.

[1]This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

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Date submitted: 02 Nov 2015 Electronic form version 1.4