Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

A comparison in activity between transition-metal oxides and transition metals ALEKSANDRA VOJVODIC, Stanford University, FELIX STUDT, FRANK ABILD-PEDERSEN, THOMAS BLIGAARD, SLAC National Accelerator Laboratory, JENS NØRSKOV, Stanford University — Transition-metal oxides are widely used materials in catalysis as substrates and promoters, but also as the active catalyst materials themselves. We compare the reactivity of transition-metal oxides with the one of transition metals. The comparison is exemplified for the ammonia synthesis reaction. First we show that there exist characteristic Brønsted-Evans Polanyi (BEP) relations (linear relations between transition state and dissociation energies) for dissociation of molecules on transition-metal oxides in the rutile and perovskite structure. It is well-known that the (211) metal surface is several orders of magnitude more reactive than the (111) metal surface due to the lower BEP line for the 211 facet. We find that both rutiles and perovskites follow BEP relations that are lower than the one of the 211 facet. Second we utilize the established BEP relations together with calculated adsorption energetics in a micro-kinetic model to obtain a volcano plot for the catalytic activity. We find that oxides have a higher turn over frequency as compared with metals. Hence, oxides intrinsically have a great advantage in terms of catalytic activity which opens up for catalyst design.

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Date submitted: 12 Dec 2011 Electronic form version 1.4