Predicting the Catalytic Reactions using Random Phase Approximation J. YAN, SUNCAT Center for Interface Science and Catalysis, SLAC, Stanford University, T. OLSEN, J.J. MORTENSEN, K.W. JACOBSEN, K.S. THYGESEN, Center for Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark, F. ABILD-PEDERSEN, J.K. NORSKOV, SUNCAT Center for Interface Science and Catalysis, SLAC, Stanford University — Density functional theory has became the workhorse for simulations of catalytic reactions and computational design of novel catalysis. The generally applied semi-local exchange-correlation functionals have successfully predicted catalytic reaction trends over a variety of surfaces. However, in order to achieve quantitative predictions of reaction rates for molecule-surface systems, in particular where there is weak Van der Waals interactions or strong correlation, it is of vital importance to include non-local correlation effects. The use of random phase approximation (RPA) to construct the correlation energy, combined with the exact, self-interaction free exchange energy, offers a non-empirical way for accurately describe the adsorption energies [1] and dispersion forces [2]. We have recently implemented RPA in the GPAW code [3-4], an electronic structure package using projector augmented wave method and real space grids. In this talk I will present our initial results comparing RPA and generalized gradient functionals for the activation energies and reaction energies for transition metal or metal oxide surfaces.

[1] L. Schimka, et.al, Nature Mat. 9, 741 (2010) [2] T. Olsen, et.al, Phys. Rev. Lett. 107, 156401 (2011) [3] J. Yan, et.al, Phys. Rev. B 83, 245122 (2011). [4] J. Yan, et.al, Phys. Rev. Lett. 106, 146803 (2011).

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