

Hybrid Hartree-Fock/density functional theory studies on ceria supported vanadia catalysts

Supported vanadium oxide catalysts are exceptionally active and selective for a large class of oxidation reactions. A representative of this class of reactions is the oxidation of methanol to formaldehyde important for chemical industry. The presence of ceria as a support material drives the commonly applied vanadium oxide catalyst to exceptionally high activity, which is well known but not yet fully understood. The previous period of the project has shown a systematic trend when comparing results obtained from semilocal density functional theory (DFT), DFT+ U , as well as Hartree-Fock/DFT hybrids. However, benchmark studies, which included dispersion effects on the energetic description of these complex rare-earth and transition metal-oxides indicated clear improvements of results when compared to experiment. Since our findings are along the same lines as work published in the literature^{1,2} for different systems important in heterogeneous catalysis, we will continue and extend previous DFT studies with particular emphasis of dispersion in *e.g.* oxygen defect formation, formation of transition structures *etc.* in course of the above mentioned vanadia catalyzed methanol oxidation. This is done having the aim in mind to provide more accurate energetics very likely leading to results of much higher predictive efficiency.

1. C. Tuma and J. Sauer, Phys. Chem. Chem. Phys. **8**, 3955 (2006).
2. S. Tosoni and J. Sauer, Phys. Chem. Chem. Phys. **12**, 14339 (2010).