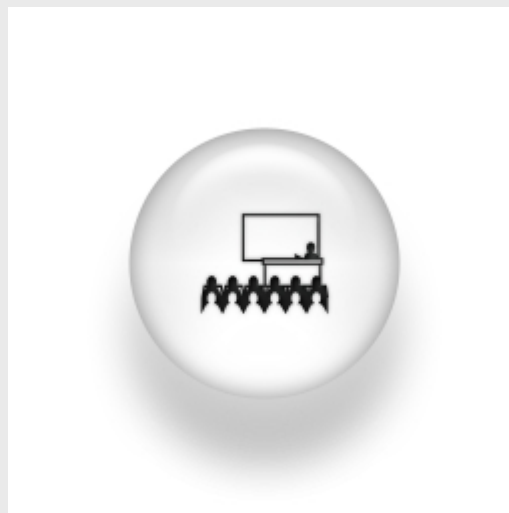


The effect of the supporting oxide on the activity of vanadia catalysts

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ABSTRACT:

As the pressure and materials gaps between real catalysis and traditional UHV single crystals studies are narrowing, experiments and modelling that straddle both sides of the gap appear essential to understand surface properties and functions of catalysts. The strong influence of the oxide support on the catalytic activity of vanadium oxides (VO_x) in oxidation reactions is well-known, yet not understood. Here, I will report theoretical models of VO_x/Al₂O₃ as well as of VO_x/CeO₂(111). These case studies were investigated using density functional theory-based calculations and statistical thermodynamics. I will show that the results obtained for the computational models for VO_x/support systems are consistent with the experimental knowledge for powder catalysts and experimental model catalysts and thus help to bridge the gap between them.

The high catalytic activity of vanadia supported on ceria as compared to alumina is discussed on the basis of the relative ease of reduction of vanadia, ceria and alumina. If time permits, I will discuss the self-assembly of nanosized Au chains on an ultrathin alumina film; a model system of another class of oxidation catalysts, namely, oxide supported (noble) metal particles.