

Understanding the electronic structure of catalysts

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Understanding the electronic structure of catalysts is a condition for the understanding of the catalytic property of catalysts. Various methods can be used to probe the electronic structure, for instance, XPS, UPS, XAS, and EELS. The core-level EELS and XAS are related to the unoccupied density of states above the Fermi level. Due to the high localisation of the core level states, core-level EELS reflects the local density of states at the site of the excited atom. Another way to understand the electronic structure is the *ab-initio* band-structure calculations (BSC). In the present work, we use EELS and BSC to study the electronic structure of various single-valence vanadium oxides. A chemical shift of the vanadium *L*-edge to lower energy-loss is observed as the oxidation states of probed vanadium decreases. BSC indicates the slight shifts of the Fermi level with decreasing oxidation state and a change of the fine structures within the O *p*-band. EELS reveals the spectral intensity of e_g^* and t_{2g}^* on the oxygen *K*-edge, with a decreasing of t_{2g} intensity as the oxidation state of vanadium increases. BSC reveals that crystal field splits the vanadium 3d orbitals into t_{2g}^* states in the lower and e_g^* states in the upper energy range of the conduction band and confirms that independent of the distortion of the octahedron units in the vanadium oxide systems, both contributions e_g^* and t_{2g}^* are visible in the density of states. For V_2O_5 , due to the V $3d_{xy} - Oc\ 2p_x/2p_y$ hybridization, BSC predicts a splitt-off of the V 3d conduction band,. This is confirmed by high-energy resolution EELS and XAS on single crystal V_2O_5 .