**ZnO interfaces: Defects, heterostructures and surface chemistry**

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In many applications, such as electrodes and thin films in heterogeneous (photo/electro)catalysis, solid-state sensors, and batteries, the surface chemistry of ZnO is crucial. Defects are known to significantly influence the physicochemical properties of ZnO. Lattice vacancies and adsorbed surface species, originating from the synthesis, can modify and inhibit the intrinsic ZnO properties. Here, we present results on the interfacial properties of nanostructured ZnO prepared by commonly employed wet-chemical methods, providing molecular evidence of the role of defects and precursors on the ensuing surface chemical properties. We provide molecular evidence of two opposing effects on the catalytic activity that occur during heat-treatment of ZnO in oxidizing conditions: Reduction of site-inhibiting synthesis residues (increasing the reaction rate), and reduction of active lattice defect sites (decreasing the reaction rate). We show that by careful “engineering”, the ZnO interface can be purposefully adjusted to control which kind of defects that are exposed and remove unwanted synthesis residues.[1]

Further, we show that by controlling the ZnO interface properties, Cu-Zn oxide heterojunction can be prepared by photo-decomposition of the chelated Cu(II) species [Cu(EDTA)]2+resulting in photocatalysts with markedly enhanced activity compared to corresponding Cu-Zn oxide structures containing a higher concentration of defects and synthesis residues.[2]  The results are attributed to more efficient electron-hole separation in purposefully synthesized Cu2O@ZnO due to well-developed interfaces.

Our results show the importance of careful synthesis and pre-treatment methods to prepare ZnO materials with desired interfacial properties for catalytic and optoelectronic applications.

[1] Fredric G. Svensson, Erik Djurberg, Seohan Kim, Gunnar Westin, and Lars Österlund, *Effect of surface impurities and lattice defects on the photocatalytic activity of ZnO nanoparticles*, in manuscript.

[2] Fredric G. Svensson, Erik Djurberg, Yige Yan, Seohan Kim, Jiri Henych, Jakub Tolasz, Frederic Dappozze, Stephane Parola, Chantal Guillard, Bozhidar I. Stefanov, and Lars Österlund, *Preparation of copper-zinc oxide pn-heterojunction catalysts by photo-deposition of [Cu(EDTA)]2+ complexes over ZnO nanorods with well-developed interfaces*, submitted.