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Reactive surface sites at metal oxide nanoparticles: From fundamental studies to potential medical application

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The ubiquity of oxides in dispersed form has prompted research strategies in two directions: understanding the existing materials by means of appropriate reference systems and tailoring the desired properties through innovative syntheses. In this talk, author will show examples of two prototype oxides, ZnO and MgO, to which extent they can be used as model systems for probing surface reactivity. When studied in parallel with DFT calculations, surface hydroxylation, provided either by adsorbing H_2O or H_2, turned to be a win-win combination for precise surface site identification. In that manner, we have demonstrated that ZnO nano-powders behave as multi-facet single crystals involving (10-10), (11-20), (0001) and (000-1) surfaces with the polar orientations corresponding to 25% of the total surface area. Moreover, we were able to report on water structures on ZnO(11-20) for the first time. Similarly, combining DFT and H_2-infrared spectroscopy on MgO nanocubes, we proposed a model in which multisite dissociation of hydrogen is suggested to occur on mono- and di-atomic steps at (001) MgO surface. Nanoparticles of a well-defined size, shape, and surface termination are required for studying the reactions occurring over their surface. A strong emphasis in our work is, therefore, given to govern the synthesis pathways when producing desired nanoparticles, either in pure or doped form. Accordingly, an example of ruling the particles surface termination by controlling synthesis parameters will be presented in this talk. Finally, author will also show how the interactions between water and nanoparticles surface can be used for studying particles dissolution as a function of their size. This is especially important in case of mixed form of ZnO and MgO (ZnMgO) which exhibits a promising potential for medical applications as an alternative to existing antibiotics.

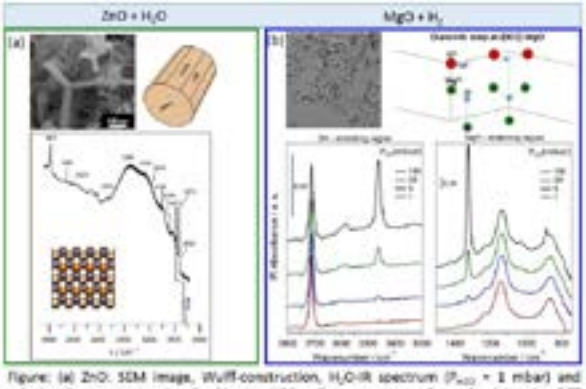

Figure: (a) ZnO: SEM image, Wulff-construction, H_2O-IR spectrum (P_{H2O} = 1 mbar) and calculated spectra associated with the H2O adlayer structure determined by the DFT approach for the ZnO(000-1). (b) MgO: TEM image, representation of a diatomic step at (001) surface with adsorbed H-atoms and H_2 IR-spectra at different P_{H2}.

Biography

Slavica Stankic has her expertise in synthesis and surface characterization of pure and multi metal oxide nanoparticles. After few years of experience of nanomaterials research from well-known international institutions (TU Vienna, Austria; INSP-CNRS, Paris, France), she has established new pathways for determining reactivity of surface sites or improving surface doping. Beside fundamental studies that involved photo-induced processes on oxide surfaces with a strong focus on the effects of particles size, shape and/or surface termination, she furthermore developed an interdisciplinary-based research project. Herein, metal oxide nanoparticles are used as model systems for studying their interaction with living organisms with a goal to assess their potential for medical applications as an alternative to existing antibiotics.

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