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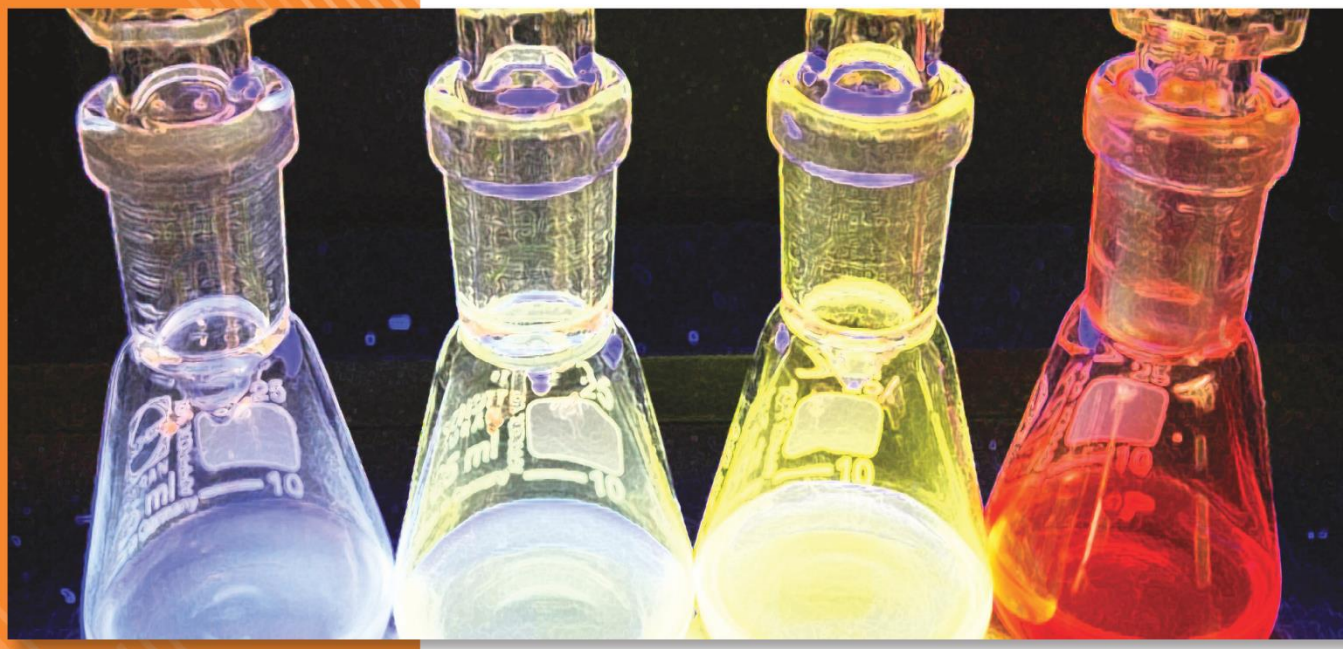

Band Gap Engineering and Defect Design of Metal Oxides using Molecular Layer Deposition

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The application of Molecular Layer Deposition (MLD) for preparation of highly photoactive thin films that can be prepared on macroscopic as well as on nano-scale substrates is relatively new. The use of hybrid organic-inorganic thin films prepared by MLD is a versatile route for attaining oxygen-deficient Titania with control over the electronic defect states and electronic bands positions. The use of MLD in the context of photocatalysis opens new routes towards non-stoichiometric oxides for tuning and optimizing the reactivity and performances of MO catalysts. MLD thin films allow the introduction of oxygen vacancies (OV) for tuning the reactivity of MOs by introduction of new electronic states within the band gap (BG). In addition, OV often function as adsorption sites for Lewis acids and bases making them surface active sites for heterogeneous catalysis. OV design offers additional valuable handles for optimizing MO electronic structure further to control over the crystalline phase and impurity doping. The correlation of OV details and band positioning with the unique photocatalytic performance demonstrated for thin films prepared by MLD will be discussed. Those systems exhibit activities that are not typically attainable by Titania. The electronic structure, charge transport, and surface properties of $TiO_{2-\delta}$ prepared by MLD are closely related to the details of the defects and OV. I will outline in my talk the implications for electronic structure design and for photocatalytic performance and our current understanding of the electronic structure evolution when annealing Ti-EG films prepared by MLD at different temperatures.

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Campus Freudenberg
Hörsaal FZH3

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