# Simulation of Oxide Nanostructures for Energy Conversion

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The design of usable and photocatalysts for efficient conversion of sunlight to hydrogen from water is a formidable task that has been approached at various levels in recent years. Conventional photocatalyst electrodes such as titanium dioxide can operate with high efficiency under ultraviolet irradiation, but it remains a challenge to drive them with visible light. Many attempts at adjusting the semiconductor band gap, generally through doping, have been made in the past, but this often leads to electron and hole trapping. One possible approach to overcome this challenge is the synthesis of nanostructured electrodes in which photon propagation and charge transport are orthogonalized, which can be realized through wire arrays or other nanostructures with large surface-to-volume ratios.

In our work we have performed hybrid density functional theory calculations of hollow $SrTiO_3$ nanotubes with the goal to identify the most stable single- and multi-walled structures. We found, e.g., that stable single-walled nanotubes, which show a widened band gap relative to the bulk, can be folded from $SrTiO_3$(110) nanosheets of rectangular morphology[1]. We recently extended this study to an investigation of various defect structures with cationic and anionic dopants[2] and found that the electronic structure of both $TiO_2$ and $SrTiO_3$ nanotubes can be modulated remarkably by substitutional impurity defects. These and other related results pertaining to inhomogeneous oxide systems in one and two dimensions will be discussed in this presentation in more detail.

References

1. S. Piskunov and E. Spohr, J. Phys. Chem. Lett. **2**, 2566 (2011)
2. S. Piskunov, D. Bocharov, O. Lisovski, J. Begens, Z. F. Zhukovskii, M. Wessel and E. Spohr, submitted to PCCP.