CHYN MEETS HARBOR

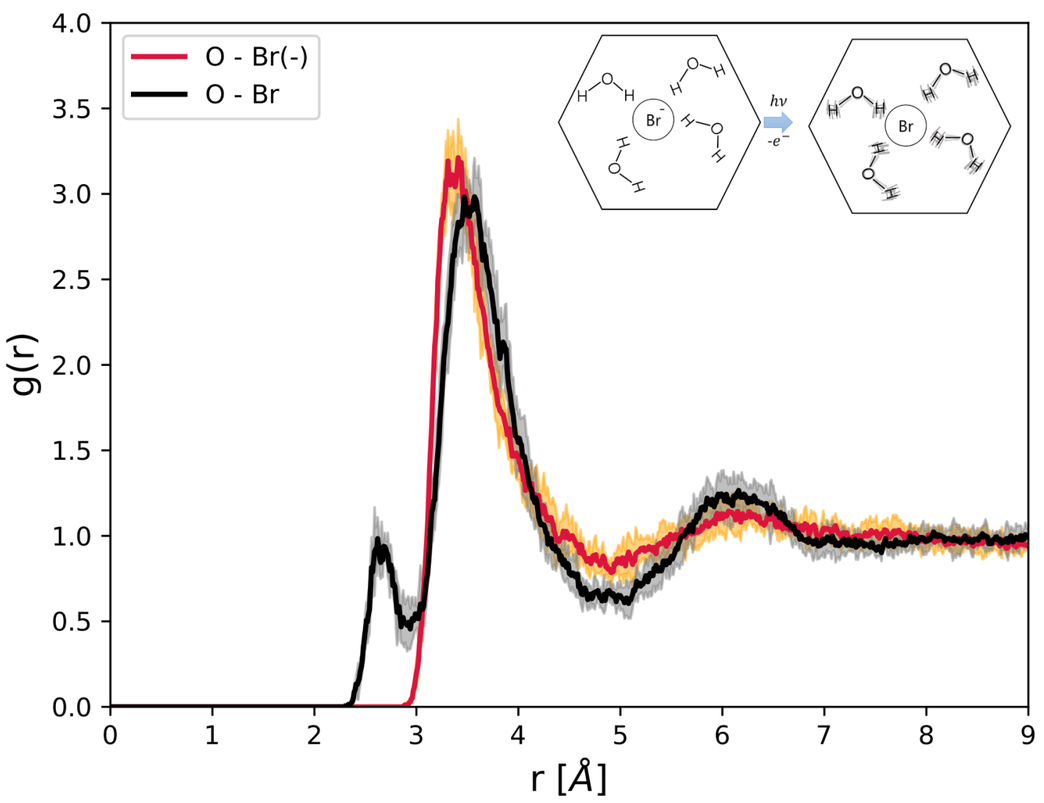
Nonequilibrium aqueous solvation around nascent bromine atoms

Dr. Marco Reidelbach

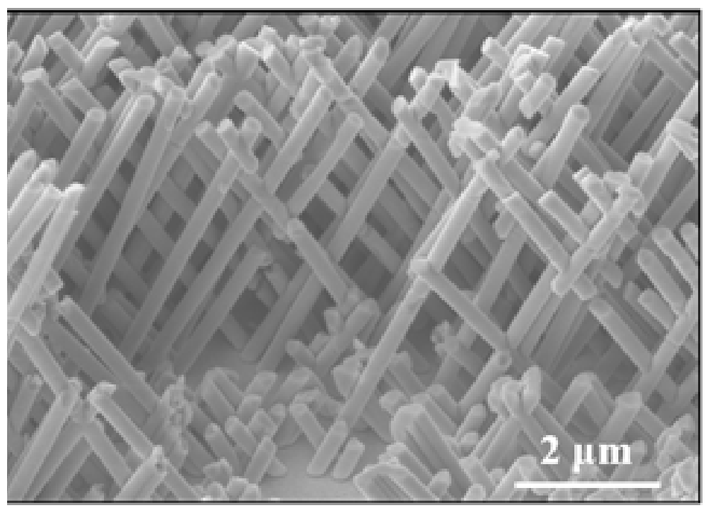
Metal-oxide semiconductors for photo-electrochemical water splitting: nanostructures or thin-films?

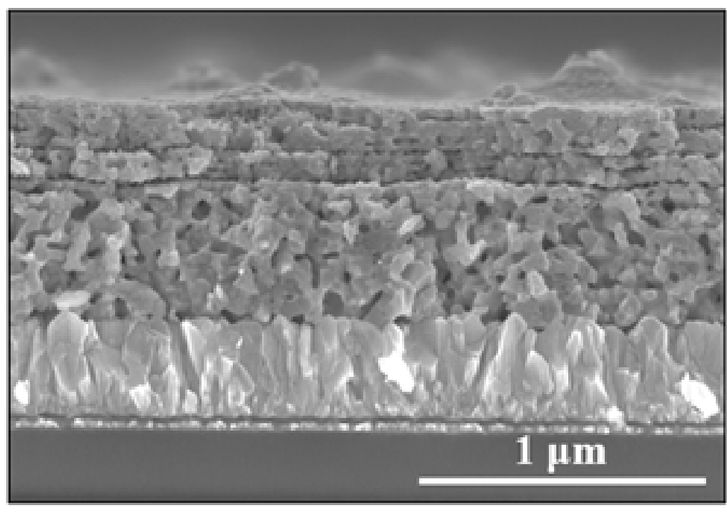
Dr. Francesco Caddeo

Abstract Talk 1: Electron transfer is a crucial step in many processes in biology and catalysis. Recent advances in time-resolved spectroscopy made it possible to investigate the nonequilibrium dynamics of the environment affecting, i.e. perturbing and/or modulating, the electron transfer. Here, we study the detachment of an electron from a bromide ion in aqueous solution as a simple model for nonequilibrium solvent affects, using mixed quantum mechanical / molecular mechanical simulations. Following the electron removal, we observe a re-arrangement of the hydration shell and the formation of a Br-H2O complex. These results are in good agreement with other experimental and theoretical work and provide an ideal starting point for investigations with an increased complexity.



Abstract Talk 2: Tuning size and shape of nanomaterials is one of the most used strategies in catalysis and photocatalysis, mainly due to the desire to obtain larger surface areas and exposure of specific crystal facets, which likely lead to enhanced reactivity. However, when studying a photocathode or a photoanode to be used in a photoelectrochemical (PEC) cell, many other parameters need to be taken into account, such as light absorption depth, minority carrier diffusion length, thickness of the space charge region, band-banding, defects concentration, electron-hole recombination rate, etc. which are interrelated and govern the PEC properties of the material. For example, while size and shape control at the nanoscale might help with decoupling light absorption depth and minority carrier diffusion length, the increased concentration of surface defects might enhance electron-hole recombination, leading to lower photocurrents. In this talk, I will discuss some of these issues while presenting results from two case-studies: p-Cu2O nanowires (left figure) and p-CuBi2O4 thin films (right figure), which are both attractive candidates to be used as light harvesting materials in the cathodic compartment of a PEC cell for the hydrogen evolution reaction.





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04.05.2021
1:15 pm | Zoom

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