

# COMPUTATIONAL SCREENING OF SOLAR ENERGY MATERIALS

Karsten W. Jacobsen

*CAMD, DTU Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark*

In the talk, I shall describe computational efforts to identify new semiconductors for efficient light absorption with special focus on materials for water splitting. The materials have to obey a number of criteria in order to work depending on the design of the water splitting device. I shall discuss relevant computational descriptors related to stability, appropriate bandgap and bandstructure, and defect-tolerance of the materials.

The potential material space of light absorbers is enormous and different approaches of how to tackle this challenge will be discussed. I shall show examples of screening studies limited to already synthesized materials or to certain classes of materials. Finally, I shall discuss new machine learning efforts to speed up identification of tailored materials.