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Abstract for an Invited Paper for the MAR16 Meeting of the American Physical Society

Predicting materials for solar energy conversion: ab-initio spectroscopy of heterogeneous interfaces GIULIA GALLI, University of Chicago

We will discuss some progress in predicting materials for solar energy conversion using ab initio calculations, in particular we will focus on heterogeneous interfaces between photo-electrodes and water and between nanocomposites. We will also address the problem of building much needed tighter connections between computational and laboratory experiments.