

Abstract Submitted
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Si-Based Earth Abundant Clathrates for Solar Energy Conversion¹ YUPING HE, Department of Chemistry, University of California, Davis, GIULIA GALLI, Institute for Molecular Engineering, The University of Chicago — We show that recently synthesized Si-based clathrates[1], composed entirely of Earth abundant elements are promising materials for solar energy conversion. Using ab initio calculations we found that the type I clathrate $K_8Al_8Si_{38}$ exhibits a quasi-direct band gap of $\simeq 1$ eV, which may be tuned to span the IR and visible range by strain engineering. We also found that electron and hole states generated by photon absorption are spatially separated on different cages in the material, with low probability of charge recombination. Finally, we computed electron and hole mobilities and obtained values much superior to those of amorphous silicon and approximately six and ten time smaller than those of crystalline silicon.

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