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Beyond Silicon: Accelerated Discovery of Sustainable Solar Energy Materials

The materials selection criteria for solar energy conversion include the chemical (e.g. abundance, toxicity, stability, scalability) and physical (e.g. bandgap, absorption, doping density, contact behaviour) properties of the underlying compounds. Many non-conventional crystalline materials are currently being investigated, including oxides (e.g. Cu2O) and sulfides (e.g. SnS); however, none are close to reaching their theoretical potential as defined by the detailed balance limit [1].

I will discuss the latest advances in materials theory and simulation [2] for the discovery of new materials for solar energy conversion. The role of predictive simulations can vary from high-throughput screening of candidate compounds, rigorous assessment of physical responses, to the optimisation of device architectures. Particular attention will be paid to origins of non-radiative electron-hole recombination that limits the performance of new technologies. Examples will be taken from our exploration of kesterite (e.g. Cu2ZnSnS4), perovskite (CsPbI3), and antimonselite (Sb2Se3) systems [3-5].

[1] "Emerging inorganic solar cell efficiency tables (Version 2)" J Phys Energy (2021); https://iopscience.iop.org/article/10.1088/2515-7655/abebca

[2] â€œMachine learning for molecular and materials scienceâ€• Nature 559, 547 (2018); https://doi.org/10.1038/s41586-018-0337-2

[3] "Upper limit to the photovoltaic efficiency of imperfect crystals from first principles" Energy Environ. Sci. 13, 1481 (2020); https://doi.org/10.1039/D0EE00291G

[4] "Lattice strain causes non-radiative losses in halide perovskites" Energy Environ. Sci. 12, 596 (2019); https://doi.org/10.1039/C8EE02751J

[5] "Rapid recombination by cadmium vacancies in CdTe" ACS Energy Lett. 6, 1392 (2021); https://dx.doi.org/10.1021/acsenergylett.1c00380

Aron Walsh holds the Chair of Materials Design at Imperial College London. He was awarded his PhD in Chemistry from Trinity College Dublin (Ireland), completed a postdoctoral position at the National Renewable Energy Laboratory (USA), and held a Marie Curie fellowship at University College London (UK). He began his independent research career at the University of Bath where he held a Royal Society University Research Fellowship. His research combines technique development and applications at the interface between solid-state chemistry and physics. He was awarded the EU-40 prize from the Materials Research Society for his work on the theory of solar energy materials, as well as the 2019 Corday-Morgan Prize for his contributions to computational chemistry. He has featured in the Clarivate Highly Cited Researchers List since 2018 and is Associate Editor for Journal of the American Chemical Society covering energy materials and machine learning.