

第293回応用セラミックス研究所講演会

293nd MSL Lecture

Date/Time: 15:00-16:00, Friday, July 3rd

Venue: Lecture Hall, Genso Cube

Speaker: Prof. Aron Walsh

Centre for Sustainable Chemical Technologies and Department of Chemistry, University of Bath, UK

Title: Emerging materials for solar energy: herzenbergite, kesterite, perovskite and beyond

Abstract:

There are a large variety of materials being developed for application in solar cells. The majority are based upon naturally occurring minerals (so-called solar mineralogy). The general procedure has been to take a multi-component system and tune the chemical composition to optimise optical absorption for the terrestrial solar spectrum. Other factors also determine whether a material can be practically employed in a photovoltaic or photoelectrochemical system, for example, the absolute band energies (work functions), defect physics, and chemical stability. I will discuss our recent progress into computing these performance descriptors from materials simulations [1-5], including advances in structure-property relationships in the kesterite (e.g. $\text{Cu}_2\text{ZnSnS}_4$) and perovskite (e.g. CsSnI_3 and $\text{CH}_3\text{NH}_3\text{PbI}_3$) families, in addition to the herzenbergite (SnS) system. New directions in the field, including the development of novel photoferroic materials, will also be addressed.

[1] "Kesterite Thin-Film Solar Cells: Advances in Materials Modelling of $\text{Cu}_2\text{ZnSnS}_4$ " Advanced Energy Materials 2, 400 (2013)

[2] "Band alignment in SnS thin-film solar cells: Origin of the low conversion efficiency" Applied Physics Letters 102, 132111 (2013)

[3] "Atomistic origins of high-performance in hybrid halide perovskite solar cells" Nano Letters 14, 2584 (2014)

[4] "The dynamics of methylammonium ions in hybrid organic-inorganic perovskite solar cells" Nature Communications 6, 7124 (2015)

[5] "Ferroelectric materials for solar energy conversion: photoferroics revisited" Energy & Environmental Science 8, 838 (2015)

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