Multi-Scale Simulations of Point and Extended Defects in Thin-Film Solar Cells

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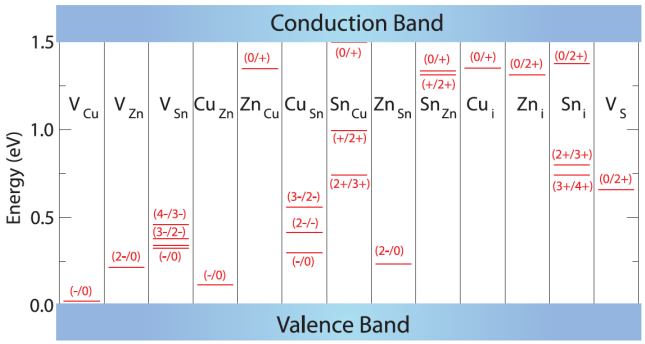
Supervisor Credentials: Walsh (*h*-index 40) has extensive experience in electronic structure simulations of thin-film photovoltaic materials (e.g. CIGS, CdTe, CZTS, Perovskites). Morgan (*h*-index 21; a new Royal Society Research Fellow) has experience in large-scale simulations of ionic transport (drift & diffusion) and microstructure.

Related 2014 Publications: (Walsh) Atomistic Origins of High-Performance in Hybrid Halide Perovskite Solar Cells (*Nano Letters, 2014*); **(Morgan)** Relationships Between Atomic Diffusion Mechanisms and Ensemble Transport Coefficients in Crystalline Polymorphs (Physical Review Letters, 2014).

CDT Strategic Alignment: A general problem with developing *new* materials for photovoltaics is that while a bulk material may appear to fulfil the requirements for an ideal absorber (e.g. band gap, optical absorption, semi-conductivity), the actual performance of thin-films may be lower than expected. For example, in less-mature chalcogenide solar cells (e.g. Cu_2S, Cu_2ZnSnS_4, $CuSbS_2$) the open-circuit voltages are less than half the value of the bandgap and limit the power conversion efficiency. Knowledge of the role of defects in these materials is crucial for optimising their performance.

Context: Point defect centres are *relatively* well characterised in $Cu(In,Ga)Se_2$ and CdTe, and we provided the first insights into Cu_2ZnSnS_4 and perovskites (see ionisation potentials for CZTS on the right). The role of grain boundaries remains controversial in the first two technologies, and almost nothing is known regarding the latter two.



PhD Project: We will develop an *open-source* materials modelling programme (in Python) for simulating point and extended defects in photovoltaic materials. The first module (year 1) will take defect formation energies and ionisation potentials (either calculated or experimental) and solve the carrier concentrations & Fermi level self-consistently. The second module (years 2-4) will construct grain boundaries, starting from an experimental or computed crystal structure, which can be used to simulate structure patterns and as a starting point for first-principles & interatomic potential calculations. The prototypes will be CdTe, Cu_2ZnSnS_4 and $CH_3NH_3PbI_3$, which will benefit from significant existing *SUPERSOLAR* activity. A complimentary experimental programme at Loughborough University (one joint APL published in 2014 on CdTe) will identify preferential orientations and morphologies. The final code and methodology will constitute a valuable community resource.