2021_06: Data-driven mineral-inspired solar energy conversion

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The Sun is an abundant natural source of clean power; however, we need better materials that can absorb sunlight and convert into electricity (solar cells) and a storable chemical feedback (solar fuels). The majority of candidate compounds are based upon naturally occurring minerals. The study of solar minerology has included kesterites ($A_2BCX_4$), perovskites ($ABX_3$) and spinels ($AB_2X_4$). The typical procedure is to take a multi-component mineral and tune the chemical composition to optimise optical absorption for the terrestrial solar spectrum.

We aim to go beyond an empirical trial-and-error approach to accelerate the discovery of candidate materials that meet the criteria for commercialisation. This is necessary to meet the UK target of net zero carbon emissions by 2050. The key area of focus will be on wide bandgap materials (500 – 700 nm) that can produce single-junction solar cells with an operating voltage (> 1 V) that is sufficient to drive challenging chemical reactions (e.g. water splitting and CO$_2$ reduction). The project will have three main stages:

1. Database building;
2. Materials modelling;

Stage 1 will involve building a database of known mineral structure types.

Stage 2 will involve populating the database with relevant chemical and physical properties from the literature and using the latest tools in quantum mechanical materials modelling.

Stage 3 will focus on deriving structure-composition-property relationships using statistical tools from the artificial intelligence community (convolutional graph neural networks), which can be used to rapidly screen larger chemical spaces. The outcome of the project will be a toolkit and methodology for data-driven screening (Walsh), while the candidate compounds will be tested in a feedback loop with experimental research (Eslava).

The project is suitable for a student with a background in chemistry, physics, or materials engineering with an interest in computers and modelling. Related reading:


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