High-throughput computational design of heterojuctions for electronic devices

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"The interface is the device" - H. Kroemer

Interfaces are ubiquitous, essential components of almost every conceivable functional material. From diodes, to photovoltaics to permanent magnets the interface region between different materials is critical to the success or failure of many of today's most important

Introducing the devil

"The surface was invented by the devil" - W. Pauli

Understanding, predicting and controlling interface properties is as challenging as it is important. To construct accurate models of interfaces we are faced with all of the challenges of bulk materials with the added complexity of having to understand how the materials form a junction and how this junction affects atomistic and electronic properties.

We have developed a procedure, based on inexpensive screening steps to identify promising interface pairings, for application in electronic devices. The method screens based on electronic matching, lattice matching and site matching; we call it ELS [1].

Electronic match

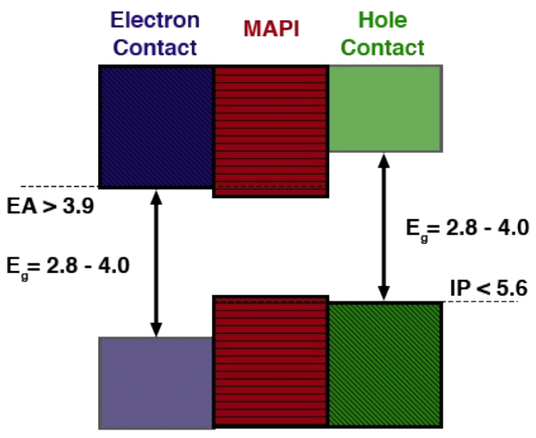


Figure 1 an example of the application of Anderson's rule for electronic matching to the popular photovoltaic absorber $CH_3NH_3PbI_3$. The IP/EA of contact layers is compared to $CH_3NH_3PbI_3$ for screening of candidates.

Depending on the application different types of band alignment are desired. One simple estimation of the band offset at a heterojunction is Anderson's rule [2], which states that the vacuum levels of the two semiconductors on either side of the heterojunction should be aligned. We are building up a database of measured and calculated ionisation potentials and electron affinities, so we can quickly scan for desired

Taming the devil

"Who holds the devil, let him hold him well" - J. W. Goethe (Faust)

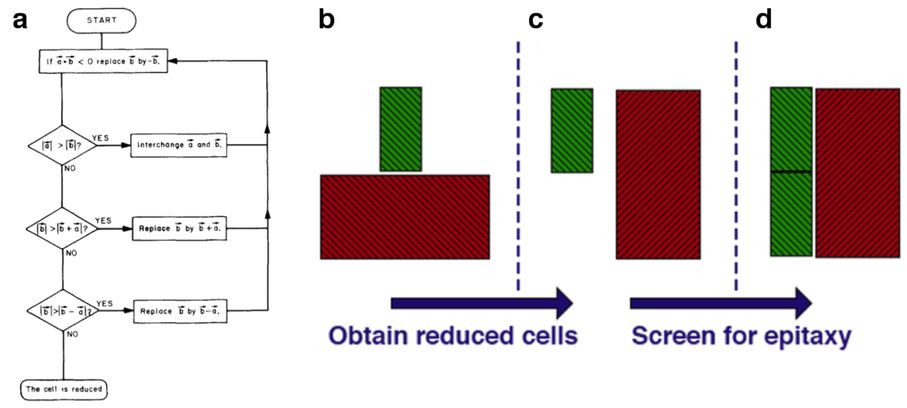
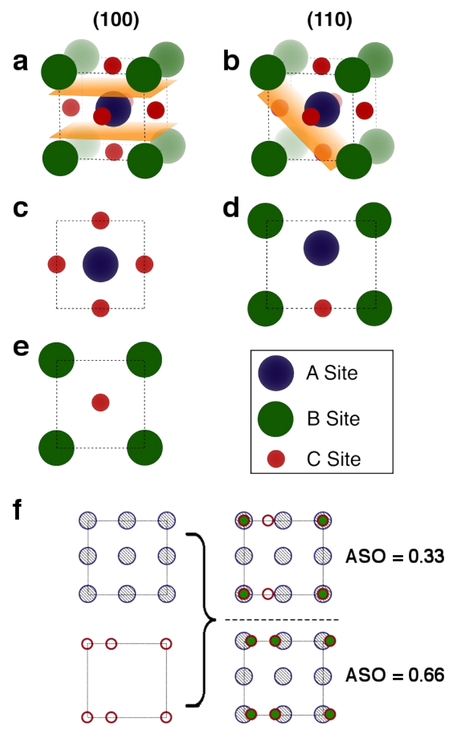


Figure 2 (a) The algorithm from the paper of Zur and McGill [3] for ensuring minimal surface vectors are used. (b-d) A schematic example of the algorithm in action.

Lattice match

We start by identifying miller indices that have epitaxial relations between the two materials. At this stage we only need to consider lattice parameters, so the screening process is extremely quick. The algorithm for identifying unique matched surface vectors is taken



Structure match

We next introduce details about the atomistic structure and bonding pattern at the interface. We use METADISE [4] to cleve all unique non-polar surfaces identified from the lattice match. We then identify the under-coordinated atoms at the surfaces. By superimposing the super-cells from the lattice match we can then identify how many under-coordinated atoms from each cell can be satisfied by the interface formation. Figure 3.

Figure 3 (a,b) cleaving a perovskite lattice. (c-e) Under-coordinated sites at the (100) and (110) surface. (f) Representation of the under-coordinated sites at two surfaces and the calculation of the maximum atomic site overlap (ASO) for the pairing.

A figure of merit

We combine the above calculated factors to derive a physically motivated figure of merit for the matching of two interfaces. We use the band offset (ΔV), the lattice strain (ϵ) and the site overlap (ASO), to form the figure of merit. ELS = 100 for a material with itself. We apply this for a screening procedure (Figure

$$ELS = \frac{ASO(100 - \exp(9.2103|\Delta V|))}{1 + \epsilon}$$

Figure 4 The results of an ELS screening for contacting photovoltaic absorber $CH_3NH_3PbI_3$. The ionisation potential and electron affinity of $CH_3NH_3PbI_3$ are highlighted as red dashed lines. To the left are candidate electron transport layers, to the right are candidate hole transport layers. The band alignment diagram is shaded according to the ELS value of the candidate material, based on electronic and structural matching.

Using ELS

ELS Python code is freely available, with instructions and examples online on GitHub.
https://github.com/keeeto/ElectronicLatticeMatch

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