

Layer-projected densities of electronic states reveal defects present at the interface. What does that mean? Your solar cell will perform less optimal than it should.

## "There are defects hidden at the interface of your materials forming the photovoltaic solar cell "







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## - Quantum-mechanic calculations, HPC



From quantum mechanic electronic energy levels and bands (top), over materials categorized by their band gap (mid) to forming interface between two or more materials (bottom).

Why DFT? Despite the well-known caveats, if used properly, brings a lot of information about a particular material. Some of them outlined above.

