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

- Quantum-mechanic calculations, HPC

Background
- Climate change, large capacity of solar energy
- Search for suitable materials
- Understanding why certain materials work as solar cells and other do not

Methods
- Substrate (film termination pair)
- Add oxidation states and spin (substrate)
- Cleave surface (polarity, symmetry)
- Substrate and film thickness

Results
- 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.