

Band Structural Engineering of TiO₂ for Efficient Solar Cells - Grant
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Summary

There are no problems more immediate and important to our present and future wellbeing than the dwindling reserves of fossil fuel resources and the hazardous environmental impact of burning fossil fuels. Among various forms of renewable energy, the photovoltaic technologies that convert solar energy into electricity using solar cells, have been extensively explored, with the present solar cell market being dominated by conventional silicon solar cells (>80% market share).

The major problem that hinders extensive use of the conventional solar cell technologies is attributed to their *high cost and lengthy pay-back period*. Therefore, economically viable solar cell technologies for the future should have the following features:

- Environmentally compatible materials (non toxic and sustainable), and chemically inert (gives a long lifetime in severe environments)
- Production cost significantly lower than the conventional solar cells, this implies that they should be made of readily available materials in the thin film form, and they should be able to be produced by low-temperature deposition technologies on large areas of low-cost substrates (e.g. metal foils, glass, plastics).
- A narrow electronic band gap and quality band structure to allow more irradiance from the Sun to be converted to electricity, so as to be able to compete with the efficiency of the conventional technologies.

Crystalline TiO₂ phases (anatase or rutile) meet all but the last criteria above. In particular they are highly stable compounds, abundant in resources, cheap to make and environmentally friendly. However, due to the intrinsic wide band gap of the TiO₂ materials (3 eV for rutile and 3.2 eV for anatase), both rutile and anatase adsorb ultraviolet light, which is typically around 5% of the spectral output of sunlight in the UV region while 45% is visible light. In order to increase the spectral absorption of TiO₂ into the visible or even infrared region, it is extremely desirable to achieve significantly narrowed TiO₂ band gap (redshift), via band structure engineering by replacing some of the Ti atoms with other elements (alloying). This needs the identification of alloying elements that *can stay in the TiO₂ sublattices to cause significant red-shift in band gap*.

In order to chart a fundamental roadmap for cost-effective alloy design, we propose to carry out fundamental computer simulation of the alloying effect on

band gap structures of TiO₂ and the thermodynamic possibility of viable alloying (Effective alloying cannot be feasible, unless sublattice mixing is thermodynamically allowed). Preliminary computation shows that it is likely to make use of over 80% of the Sun irradiance for photovoltaic energy conversion, via forcing useful elements into the Ti sublattice of the anatase TiO₂. This proposed SEED CORN project aims to consolidate the preliminary findings via refined simulation, in order to lay a solid foundation for extended multi-disciplinary research and development, via close collaborations with regional and national academics and industries. *The technological importance of the proposed work is evident, as the realisation of significant redshift in the TiO₂ band gap will initiate explosive changes in the landscape of photovoltaic technologies. The overall success in the proposed band structure engineering of TiO₂ will endow the low-cost solar cell candidate with even higher efficiency (> 80% in theory) than that for the most expensive solar cells of today (~30% for single-crystal multi-junction solar cells).* This would offer major technological leverages to the Northwest and the UK, for wealth creation and clean environment, as renewable energy technologies are emerging as to play a more and more significant role in economic competitiveness. To the wider community of materials science and engineering, the methodology out of this work is fundamental for the development of various designer materials with targeted properties/functionalities.