From solar cells to biology: how materials modelling skills translate

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Abstract

As I have but recently joined the Centre for Nanoscale BioPhotonics (CNBP), I will present an overview of my background and skills before covering a recent project in more detail. I will then outline my current CNBP research activities and interests.

Dye-sensitised solar cells (DSSCs) have sparked considerable interest over two decades. Recently, a method of polymer-wire sensitisation was demonstrated; the polymer is suggested to form a hole transport pathway (wire) following initial charge separation. We predict the optical properties of this polymer in various interfacial configurations, including the effects of chain length and attachment to {100} or {101} TiO2 facets. Contrary to most DSSCs, the {100} facet model best describes the experimental spectrum, predicting a relative thickness of 5.7 □ 0.2 mm, although {101} attachment, if implemented, may improve collection efficiency. Long chains are optimal, and stable attachment sites show minimal differences to absorbance in the major solar emission (visible) band. Combinations of {100}, {101}, and pseudo-bulk TiO2 models in three- parameter fits to experiment confirm the relative importance of the {100} facet.

Bio

Daniel is a theoretical physicist based at the RMIT node of the Centre for Nanoscale BioPhotonics. He received his PhD in 2013 from The University of Melbourne for his work on the physics of low-dimensional nanostructures. Since then, he has spent two years in the Theoretical Chemical & Quantum Physics group at RMIT University, working on models across diverse topics, before joining the CNBP theory team in December 2014.