DFT studies of UV-vis spectrum and photovoltaic properties of new ruthenium complexes

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Presentation Preference: Poster

Career Level: (^) honours student

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Abstract:

Third generation solar devices rely on effective dye sensitisers which produce excitons over broad range of wavelengths of light. Much effort has been invested in discovering new dyes which are suitably stable, absorb light well and bind strongly to semiconductor surface. It is of interest to characterise dyes using computational methods in order to conserve time and minimise wasting rare metals. A recently synthesised dye, $[(\eta^6\text{-p-cymene})Ru(4,4', 5,5'\text{-}H_4tcbpy)Cl][Cl]$[1], is characterised using density functional theory (DFT) computational methods at B3LYP/LAN2DZ theory level, comparing geometry and absorption spectra to experimentally derived values. Although only preliminary results are presented, they will provide a launch pad for further novel dye discoveries; solid state calculations are yet to be performed and will further elucidate mechanisms of action for dye redox transitions and semiconductor electron injection pathways.

Reference: 1. T. Rüther, et al, J. Organomet. Chem. 823(2016)136-146.

Biographical Statement of Presenter:

Fred is currently completing an undergraduate honours thesis in chemistry as part of Professor Feng Wang's molecular model discovery laboratory (MMDL) group at Swinburne University. He has an interest in renewable energy technology, particularly in computer aided advanced materials design.

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