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DFT Studies of Fe, Ru & Os Light-Sensitive Energy Conversion Dyes/Catalysts

Metal-to-ligand charge transfer compounds, specifically the ruthenium bipyridyl complexes, are presently amongst the ideal photocatalytic compounds used, not just in the DSSC conversion of solar energy into usable electric current,[1] but also in photocatalytic reduction of both CO₂ and H₂O, towards the production of renewable H₂ fuel and CO,[2] the latter being the main reagent in the Fischer-Tropsch synthetic liquid fuel manufacturing process. Spectral and electrochemical tuning naturally lie at the basis of finding suitable dye derivatives. High performance computing lends itself ideally towards preliminary investigations, significantly narrowing down the experimental search field when seeking suitable candidates for particular applications.

[1] Pashaei, B., Shahroosvand, H., Graetzel, M., Nazeeruddin, M.K., Influence of Ancillary Ligands in Dye-Sensitized Solar Cells (Review), *Chemical Reviews*, 116/16, 2016, 9485-9564.

[2] Kuramochi, Y., Ishitani, O., Ishida, H. Reaction mechanisms of catalytic photochemical CO₂ reduction using Re(I) and Ru(II) complexes (Review), *Coordination Chemistry Reviews*, 373, 2018, 333-356.

Presenter Biography

Prof. K G von Eschwege is a lecturer and researcher at the Chemistry Department of the Free State University, with keen interest and research in - amongst others - sustainable energy applications.

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