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RESEARCH ACTIVITIES

Mechanistic Understanding of CO_2 reduction reaction by quantum chemical methods

- Electrocatalysis
- Fundamental modelling of CO_2 reduction reaction on Cu based materials
- Rational design of catalysts
- Artificial photosynthesis

SUMMARY

I am a chemical engineer with specialisation in multiscale modelling, heterogeneous catalysis and reaction engineering. My former research activities were focused on the study of multimetallic mixed oxides (MoVTeNbO) for the conversion of ethane to ethylene, and on the fundamental modelling of complex materials for Fischer-Tropsch synthesis (CO_2 resistant Fe-based catalysts).

Currently, I am working on a density functional theory (DFT) study applied to elucidate the reaction mechanism of the CO_2 reduction reaction over Cu based catalyst.

PUBLICATIONS

- Electrochemical CO2 Reduction to Ethanol with Copper-Based Catalysts. Dilan Karapinar, C. E. Creissen, J. G. Rivera de la Cruz, M. W. Schreiber, M. Fontecave. *ACS Energy Letters* 2021 *6* (2), 694-706. DOI: 10.1021/acsenergylett.0c02610

- First Principle Study on the Adsorption of Hydrocarbon Chains Involved in Fischer–Tropsch Synthesis over Iron Carbides. J. G. Rivera de la Cruz, M. K. Sabbe, and M-F. Reyniers. *J. Phys. Chem. C*, 121(45): 25052-25063, 2017, DOI:10.1021/acs.jpcc.7b05864

- First principle study of chain termination reactions during Fischer-Tropsch synthesis on χ-Fe_5C_2(010). J. G. Rivera de la Cruz, M. K. Sabbe, and M-F. Reyniers. *Mol. Cat.*, 453:55-63, 2018, DOI:10.0.3.248/j.mcat.2018.04.032

- Comparative study of chain termination and chain propagation reactions of Fischer-Tropsch Synthesis over Iron Carbides. J. G. Rivera de la Cruz, M. K. Sabbe, and M-F. Reyniers. *submitted*