



UNIVERSITY
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Department of Chemistry

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Honours projects in the Schreckenbach group, Fall 2015

1. Surface reactivity

In this project, you will apply a newly developed computational method (solvation model) to study catalytic reactions on interfaces between solution and metal or semiconductor surfaces. The purpose is to verify and apply the new methodology for modeling solvation, while, at the same time understanding important reactivity such as heterogeneous catalysis.

2. Singlet fission materials

In this project, you will use computational chemistry to study and screen potential novel singlet fission (SF) materials. SF is a process where the absorption of a high-energy photon leads to two excited electrons (two electron-hole pairs) on neighboring chromophores. It has the potential to significantly increase the efficiency of solar energy conversion. Typical SF chromophores are planar molecules with extended conjugation.

Other projects

... are possible, including

- Modeling of environmentally relevant gas-phase reactions of mercury;
- Elementary chemical processes in novel batteries;
- 2D materials;
- Actinide chemistry;
- Method and code development.

Research in my group is computational/ theoretical in nature; we develop and apply the tools of computational quantum chemistry to understand various chemical questions. See my webpages for more details, and come talk to me!

Dr. H. Georg Schreckenbach

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