Towards the multiscale modeling of catalysis

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We have embarked on a multistage research program on the multiscale theory, simulation, computation and understanding of catalysis along two lines: i) enzymes and ii) heterogeneous nanocatalysts.

Progress will be illustrated by one or more of the following projects:

I) **Electron transfer between proteins**[1]– the role of interfacial residues in governing the solvent dynamics to accelerate the electron transfer[2] including the effects of quantum decoherence[3]. The techniques involved are classical Molecular Dynamics combined with the Pathway Model of electron transfer (within Marcus theory), constrained Density Functional Theory (DFT), Born-Oppenheimer Molecular Dynamics and a new methodology for quantum decoherence.

II) **Nanocatalysts for in-situ upgrading of the oil sands** – We are working with Pedro Pereira's experimental bitumen upgrading group to help design new nanocatalysts that can be introduced to the oil sands in order to do some of the upgrading underground, leaving undesirable products in the reservoir. So far we are focusing on the hydrogenation of benzene as a model. Techniques include DFT on periodic (VASP)[4] and cluster (deMon)[5] models and a fast semiempirical method from the Miyamoto lab, UAQCMD – Ultra-Accelerated Quantum Chemical Molecular Dyamics.

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