UCL CMMP Summer Research Project 2018

Project: Investigating Charge Transfer at Heterogeneous Interfaces: Multi-heme proteins adsorbed on Au(111)

Supervisor: 1st supervisor**:** Dr Zdenek Futera (Senior Postdoc in Blumberger group)
2nd supervisor**:** Prof Jochen Blumberger

Duration: 6 weeks (from 25th June to 3rd August 2018)

Project description

Multi-heme proteins containing chains of redox heme cofactors are fascinating biomolecules that facilitate long-distance extracellular electron transport (EET) in metal-reducing bacteria. In recent experiments one of these proteins (STC) could be isolated and incorporated in a protein-monolayer tunnel junction device. Unusually high currents at modest bias-voltages were reported for this protein making it of great interest for bionanoelectronic applications. However, there is currently no theoretical understanding of the conduction mechanism across these proteins.

The goal of the proposed project is to simulate the measured I-V curves assuming either a fully incoherent charge hopping model or a fully coherent tunneling model. These models require input parameter that we propose to obtain from atomistic molecular dynamics simulation and density functional theory calculations on the protein adsorbed on Au(111) thereby modelling the experimental conditions. The outcome of these calculations and their comparison with available experimental data should give us a deeper understanding of the relevant transport mechanism in these devices.

Project schedule

Week 1: Reading literature, learning how to work with needed software (visualization with VMD, Gromacs/Amber tools to extract data from MD trajectories, scripting)

Week 2: Basic understanding of CP2K code, preparing input for coupling calculations (POD method), learning how to run calculations on HPC machines (Archer)

Week 3-4: Computing reorganization free energies from MD trajectories by provided scripts, post-processing of DFT data (visualization of molecular orbitals, electronic-state levels and band alignment on the metal/organic interface)

Week 5: Collecting computed data and simulating the I-V curves by applying different theoretical models (incoherent electron hopping vs. coherent tunneling)

Week 6: Analyzing results, writing final report, presenting the results on the group meeting

Besides the above schedule, the student will be asked to attend weekly meeting of the group.

Project outcome

By solving the proposed project the student will learn how to analyze MD trajectories by available software tools (Gromacs, AmberTools), visualization (VMD) as well as simple scripting techniques (BASH, Python). Further, the student will learn how to prepare basic input for DFT code (CP2K), run the calculation on HPC machine (Archer), extract and analyze the data. Besides these computer skills, the student will be guided how to write the final scientific report of the project and how to present obtained data to other people, which are the important soft skills needed in any research career.