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Atomic-Scale Modelling of Charge Transport Across Interfaces

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Abstract:

The charge transport across interfaces is a critical process in solar cells, batteries and other electronic devices. It is therefore important to obtain a fundamental understanding of the charge transport. In this lecture I will introduce the atomic-scale simulation of electron transport across interface using first principles methods. I will give a brief introduction to Density Functional Theory (DFT) and describe in further details the application of DFT to interface systems using the Non Equilibrium Greens Function (NEGF) method. This methodology allows for describing the electron transport across the interface in the presence of an external applied bias. The application of the methodology to interfaces in solar cell systems[1,3] and batteries[2] will be presented. Finally, I will discuss industrial application examples of atomic-scale simulations and industrial career opportunities.

References:

1. D. Stradi, M. Brandbyge, U. Pozzoni, A. Blom and K. Stokbro, /Direct and general approach for modelling metal-semiconductor interfaces using density functional theory and non-equilibrium Green's function/, Phys. Rev. B 93, 155302 (2016)
2. Mekonnen, Yedilfana S., et al. "Role of Li2O2@ Li2CO3 Interfaces on Charge Transport in Nonaqueous Li–Air Batteries." *The Journal of Physical Chemistry C* 119.32 (2015): 18066-18073.
3. K. Stokbro and S. Smidstrup, /Electron transport across a metal-organic interface: Simulations using nonequilibrium Green's function and density functional theory/,Phys. Rev. B *88*, 075317 (2013).