Abstract: Parametric flow of effective Hamiltonians in *ab initio* transport calculations

Ab initio calculations for transport properties of single molecules based on the density functional theory (DFT) often appear to fail giving a quantitative description of the conductance that is seen in available experimental current-voltage curves (I-V). However, apart from the zero bias conductance the I-V traces contain a lot more and very important characteristic information, like step positions and inelastic satellite peaks. Many such features can be analyzed in great detail by monitoring the flow of the self consistent (Kohn-Sham) Hamiltonian (or derived quantities) under a variation of model parameters. Some examples of such parameters are the chemical potential of the leads, a gate voltage, the inter-electrode distance, the number of electrode atoms kept in the DFT calculation etc.. The talk will present results of recent studies that have utilized this idea. It will be demonstrated, that this approaches can provide a quantitative understanding not only in principle, but also in practical applications. Several examples of the latter will be presented.