Cluster-based density functional approach to transport through molecular and atomic contacts

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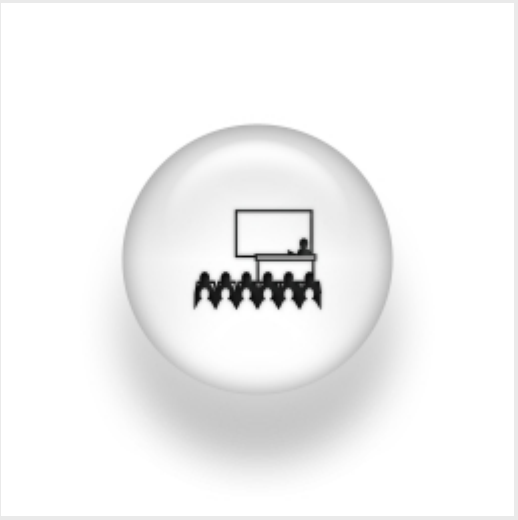
Dr. Fabian Pauly



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We present our recently developed ab-initio method to model quantum transport in atomic and molecular contacts. The electronic structure is treated at the level of density functional theory, and the parameters needed to describe transport are extracted from finite clusters. As applications, we study (i) the tilt-angle and temperature-dependent conductance of biphenyl-derived molecules, (ii) the length-dependent conductance and thermopower of oligophenylenes, and (iii) highly conductive junctions of benzene coupled directly to Pt electrodes. If time permits, we will also present recent more qualitative work on the influence of light on the current in molecular junctions.