MAR10-2009-000205

Abstract for an Invited Paper
for the MAR10 Meeting of
the American Physical Society

Electron dynamics and the approach to steady state in molecular junctions

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The description of transport through a molecular junction typically invokes the idea of a steady state - the system is driven out of equilibrium, and it is assumed that on the experimental timescale it will relax to a steady state distribution. In this talk we critically examine the approach toward steady state and address the question of whether or not there might be realistic situations where steady state never obtains. The tool we use for this study is real-time dependent density functional theory. We find that while the simulations can often show systematic deviations from reality, yet our calculations suggest that non-steady-state behavior could be relevant on ultrafast timescales.