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Tenkých vrstev a nanostruktur

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TÉMA

Simulations of electron transport phenomena in single-molecule junctions

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Single-molecule devices are ideal test beds for studying a range of quantum transport phenomena, and new insights are obtained through critical comparison between experiments and theoretical models.

In this talk I will describe how first-principles transport simulations based on density functional theory (DFT) in combination with nonequilibrium Green's functions (NEGF) can provide detailed and quantitative information. Examples include the impact of atomic-scale structure of metal-molecule interfaces on junction conductance [1,2] as well as effects of electron-vibration interactions for device characteristics and stability [3,4].

[1] G. Schull, T. Frederiksen, A. Arnau, D. Sanchez-Portal & R. Berndt, Atomic-scale engineering of electrodes for single-molecule contacts, Nat. Nanotechnol. 6, 23-27 (2011)

[2] T. Frederiksen, G. Foti, F. Scheurer, V. Speisser & G. Schull, Chemical control of electrical contacts to sp2 carbon atoms, Nat. Commun. 5, 3659 (2014).

[3] T. Frederiksen, M. Paulsson, M. Brandbyge & A.-P. Jauho, Inelastic transport theory from first principles: methodology and application to nanoscale devices, Phys. Rev. B 75, 205413 (2007).

[4] J.-T. Lü, R. B. Christensen, G. Foti, T. Frederiksen, T. Gunst & M. Brandbyge, Efficient calculation of inelastic vibration signals in electron transport: Beyond the wide-band approximation, Phys. Rev. B 89, 081405® (2014).

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