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Titel des Beitrags:  Joule heating in molecular tunnel junctions: application to C60  
Abstract:  First-principle calculations based on density functional and non-equilibrium Green’s functions are used to compute the power emitted in conducting molecular systems due to scattering with localized vibrations. The balance between the rate of phonons emitted and dissipated into the contacts allows the computation of the steady-state distribution of phonon quanta localized in the junction, from which we extract the local temperature reached by the molecule. The model includes two critical quantities; (i) the rate of phonon emitted in the junction due to electron-phonon scattering and (ii) a microscopic approach for the computation of the phonon decay rate, accounting for the dynamical coupling between the vibrational modes localized on the molecule and the contact phonons. The method is applied to the discussion of several limiting conditions and trends, depending on electron-phonon coupling, incoherent transmission and phonon dissipation rates, using both analytical results and numerical calculations.  
Stichworte:  molecular electronics, electron-vibron scattering, power dissipation, NEGF  
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