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Electron-vibration interaction in molecular electronics and GW approximation for the e-e interaction in transport theory

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The field of molecular electronics has seen a tremendous expansion in recent years, thanks to the realization of ingenious experimental setups and the fundamental achievement of reproducible results and behaviours. Significant progresses have also been made from a theoretical point of view, although the agreement with experiments is still not satisfactory. The challenges for a complete understanding of transport in such systems are still considerable. Inelastic electron tunnelling spectroscopy is becoming very popular in the field thanks to its powerful capability of probing molecular vibrational properties and could provide in the future a valuable characterization tool if correctly related to theoretical calculations. We simulate IETS spectra of various molecules between metal contacts and show the importance of such simulation for the interpretation of the experiments. Particular attention is devoted to the evaluation of Joule heating and thermal dissipation. The problem is tackled within the formalism of NEGF by the calculation of appropriate electron-phonon self-energies. The electron-phonon coupling is derived from the DFTB Hamiltonian. The Power dissipated is calculated from the virtual contact current originated from phonon emission and absorption processes. Preliminary results of thermal dissipations of molecules coupled to Au and Si substrates will be shown. As well known, all DFT methods tend to underestimate the electronic band-gap of semiconducting and insulating materials. In particular the band-gap of conjugated organic molecules is usually underestimated by few electronvolts. However, band-gap corrections are crucial for quantitatively correct calculations of the tunneling current through organic molecules. We show a novel implementation of the *GW* correction applied to our DFTB method and show its applications to molecular systems sandwiched in-between electrodes to obtain a first-principle correction of the $e - e$ interaction energy. The resulting self-energy is used to improve the system *GF* and to obtain a correction of the tunneling current. We also apply the *GW* correction in the context of the computation of the complex band-structures of polymers such as poly-acetylene or poly-phenylene and show how the energy gap and decay lengths of the evanescent states should be corrected by quasi-particle effects.