**Inelastic scattering and current-induced heating in graphene nanoconstrictions**

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## Abstract

The interplay between electronic current and phonon dynamics is an important and intriguing problem in nanoelectronics. For instance, this interaction is observed as contact disruption in graphene nanoconstrictions (GNCs), where the current-density can locally be very high, and is used for current-annealing of graphene edges [1]. Additionally, the structural response to the high bias can be studied by *in situ* transmission electron microscopy, making GNCs a good test bed for current-induced phenomena [2]. We have studied phonon dynamics in a GNC (Fig.1A) in the presence of electronic current using nonequilibrium Green's functions (NEGF) and a semi-classical Langevin equation in combination with density functional theory (DFT) calculations [3]. We will argue that current-induced forces, different from Joule heating, will severely heat up such nanostructures.

We find that the electronic transmission spectrum has several peaks with a width that is less than or comparable to typical optical vibrational frequencies of 0.2 eV (Fig.1B). We tune the Fermi-level, $E_F$, to such a resonance (marked by a square) and find that the local current path runs through the center of the device (Fig.1C). The change in current paths when changing the energy illustrates the strong dependence on the electronic energy. Consequently, the interaction between current and local vibrations also depends strongly on energy. Therefore, we find that the probability of emitting a phonon can exceed that of absorbing one due to the strong variation in symmetry of the scattering states at $E_F \pm \hbar\omega$. This manifests itself in a negative vibrational damping and density of states (Fig.2A) and a corresponding nonlinear heating (Fig.2B). The effect is robust towards including the damping from the surrounding vibrations (Fig.2B full line) and it may limit the stability and capacity of GNCs to carry high currents.

We also examine the inelastic scattering effects in the electronic current. The *IV*-characteristics can provide a spectroscopic fingerprint of localized vibrations in the system. We have recently developed a method that can include the rapid variation in the electronic spectrum with energy in inelastic tunneling spectroscopy (IETS) modelling [4]. Tuning the energy away from a resonance, the model gives results consistent with the wideband lowest order expansion (wbLOE) widely used in DFT modelling (Fig.3B). At resonance the spectrum changes quite remarkably with the novel extended LOE (exLOE) giving rise to several dip-peak features not present in the wbLOE model. Including the energy variation on the vibrational energy scale is important in electronic conductance and local heating modelling. This is especially true for graphene nanostructures where local vibrational frequencies approach 0.2 eV.

## References

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**Figure 1:**

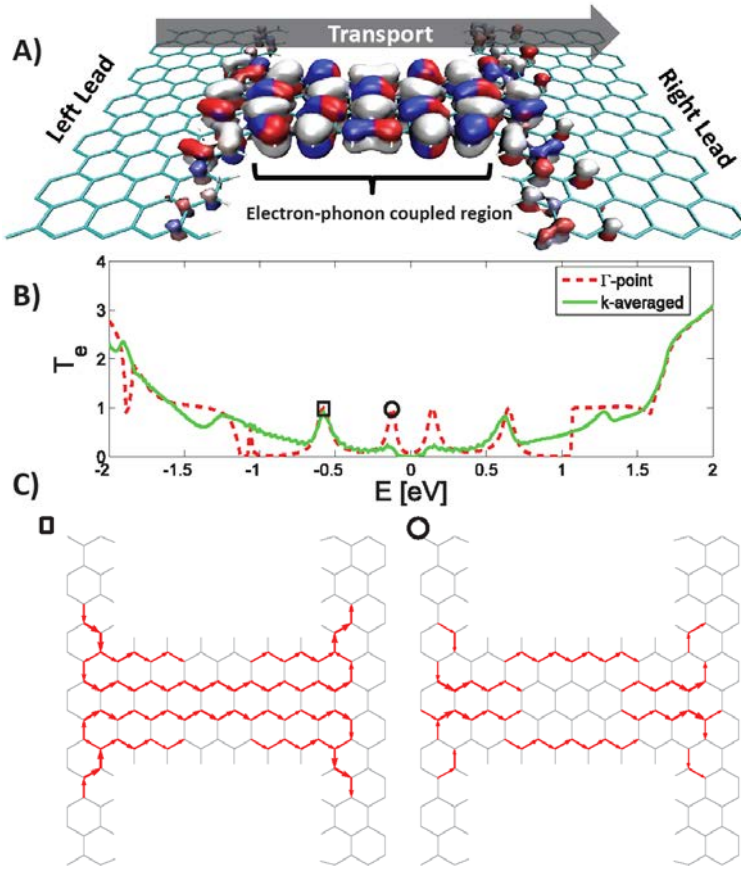


**Figure 2:**

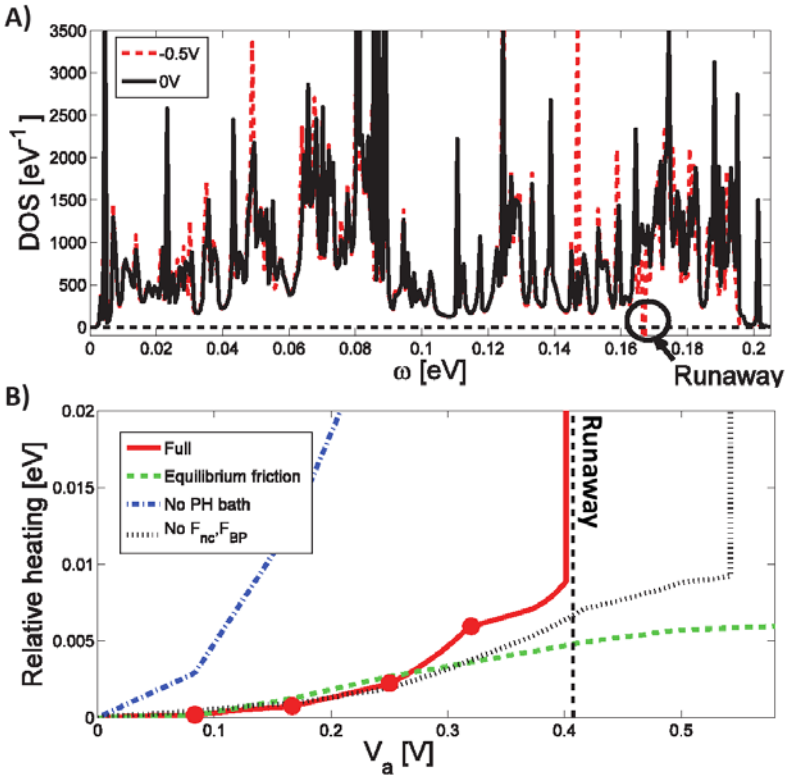


**Figure 3**