A first-principles study of current-induced forces in carbon-based nanojunctions

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In ballistic nanoscale conductors the high current density can lead to substantial changes in the atomic structure, as seen in experiments[1,2].

We calculate the current-induced forces on the atoms for different models of carbon-based nanojunctions [3] under a high applied bias voltage on the order of 1 Volt. Specifically, we have performed non-equilibrium charge transport calculations, employing first principles electronic structure and transport calculations based on density functional theory combined with non-equilibrium Greens functions (DFT-NEGF) [4].

Our findings show how the forces on the atoms are related to the chemical bonds in the junctions. In particular, we analyze how bonds get weakened/strengthened in the presence of current, and trace these effects back to the redistribution of bond charge due to the current flow [5]. Further, the role of the electric field due to the applied bias voltage and the relation between the forces and the potential drop in the junction is discussed.

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