Molecular Electronics through tunneling in 1D and *quasi*-1D devices

We have simulated electron tunneling through one-dimensional molecular junctions based on first-principles simulations using the density functional theory combined with the non-equilibrium Green's functions methodology. The bridging atom bonds weakly to the electrodes in both systems, it strongly affects the electronic transport properties, such as electron transmission, current–voltage relation, differential conductance, density of states and eigenchannels. This is demonstrated by comparing with the results obtained from the corresponding systems for both the 1D and the *quasi*-1D junctions in the absence of the central sodium atom. The revealed transport properties are sensitive to the molecular geometry. This helps future molecular electronic device design.