Identification of pristine and defective graphene nanoribbons by phonon signatures in the electron transport characteristics

Inspired by recent experiments where electron transport was measured across graphene nanoribbons (GNRs) suspended between a metal surface and the tip of a scanning tunneling microscope [Koch, Nat. Nanotechnol. 7, 713 (2012)], we present detailed first-principles simulations of inelastic electron tunneling spectroscopy (IETS) of long pristine and defective armchair and zigzag nanoribbons under a range of charge carrier conditions. For the armchair ribbons we find two robust IETS signals around 169 and 196 mV corresponding to the D and G modes of Raman spectroscopy as well as additional fingerprints due to various types of defects in the edge passivation. For the zigzag ribbons we show that the spin state strongly influences the spectrum and thus propose IETS as an indirect proof of spin polarization.