Abstract Submitted
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First-principles study of resonant Raman spectroscopy in graphite and carbon nanotubes[1] DAVID PRENDERGAST, University of California at Berkeley and Lawrence Berkeley National Laboratory, JACK DESLIPPE, University of California at Berkeley, STEVEN LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory — Resonant Raman spectroscopy is an increasingly used experimental tool for the characterization of carbon nanotubes (CNTs). It explores the coupling of optical, electronic, and vibrational modes in these quasi-one-dimensional systems. Using first-principles methods we calculate the electron-photon and -phonon matrix elements necessary to estimate the first-order Raman cross-section. For graphite, the non-interacting quasiparticle spectrum is sufficient, however, for CNTs, the excitonic spectrum and wave functions require an accurate description of electron-hole correlation. We calculate excitonic effects by solving the Bethe-Salpeter equation, using as input the quasiparticle spectrum obtained within the GW approximation to the electron self-energy. We analyze the exciton-phonon coupling in CNTs and its impact on the resonant Raman cross-section.

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David Prendergast
University of California at Berkeley (UCB) and
Lawrence Berkeley National Laboratory (LBNL)

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