# Strain-dependent dielectric screening in a carbon nanotube and electronic response of graphene to proton irradiation

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**Abstract:**

High-performance computing enables quantum-mechanical studies of material properties and, in particular, of electronic excitations with unprecedented accuracy: Many-body perturbation theory is capable of predicting electronic and optical properties in excellent agreement with experiment. Dynamics of excited electrons that interact with fast-moving ions can be investigated accurately and efficiently using real-time time-dependent density functional theory.

We use these quantum-mechanical first-principles simulations, based on the *GW*+BSE approach, to provide an accurate connection between structural and optical properties of materials: Here, we will specifically discuss how different dielectric screening contributions, e.g. due to free carriers, electronic, and lattice polarizability affect electronic and optical properties. Our first-principles calculations allow us to identify an influence of strain on electronic screening and to accurately quantify the impact on electronic structure and optical absorption of an (8,0) carbon nanotube.

Excited electronic states also dominate early stages of radiation damage: We will discuss how energetic particle radiation that can be used to change the properties of two-dimensional materials, interacts with the electronic system of the target. We apply real-time time-dependent density functional theory and Ehrenfest molecular dynamics to study a monolayer of graphene. More specifically, we compute secondary electron yield, charge transfer, energy transfer, and equilibration time-scales after impact of charged-ion projectiles. Insights from our simulations impact scientific questions related to materials design of radiation-damage-resistant materials, helium microscopy, and focused-ion beam sample manipulation and characterization.