Title: Real-time TDDFT study of electronic excitation in particle irradiated semiconductors

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Abstract:

Energetic charged-particle radiation has exciting applications including modern research, semiconductor industry, and medicine. The successes of these applications rely on quantitative understanding of fundamental interactions between particle radiation and target materials. Unlike elastic scattering between particle and target materials, quantitative understanding of electronic excitation due to ionizing particle radiation remains elusive. Recently, with the advance of high performance computing, we can now apply real-time time-dependent density functional theory to system that requires large supercell. We present our recent results of beam-sample interactions in bulk, layered, and defected semiconductors. Based on the findings, we identify interesting relations between electronic excitation, electronic structure, and particle kinetic energy, which are critical for better application of particle radiation.