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APS March Meeting 2019
Monday–Friday, March 4–8, 2019; Boston, Massachusetts

Session A15: 2D Materials (Semiconductors) -- Monolayers
8:00 AM–11:00 AM, Monday, March 4, 2019
BCEC Room: 154

Sponsoring Units: DMP DCOMP
Chair: Vinod Sangwan, Northwestern University

Abstract: A15.00006 : The Born-Oppenheimer approximation in graphene: A time-dependent perspective*

9:00 AM–9:12 AM

← Abstract →

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In graphene, electron-phonon interactions are known to play an important role in the loss of electronic wavefunction character and relaxation processes following photoexcitation. We model electronic interactions with nuclear vibrations from a microscopic, time-dependent perspective. Utilizing a time-dependent tight-binding Hamiltonian for the electronic degrees of freedom, we numerically determine the time-evolved electronic wavefunction in the presence of classical nuclei vibrating along normal modes. We examine the solutions by comparing them to those predicted within the adiabatic Born-Oppenheimer (ABO) approximation. We find that, for electronic states on energetically isolated potential energy surfaces, the adiabatic Born-Oppenheimer (ABO) approximation offers an accurate picture of time-evolution. But, in the presence of avoided crossings, the ABO approximation quickly breaks down as the electronic wavefunction becomes a superposition of ABO basis states. Moreover, electronic character is preserved over several vibrational periods for a finite lifetime, indicating highly diabatic time-evolution.

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