Modeling Defects in 2D Materials for Quantum Information Science

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Abstract: Point defects in semiconductors have emerged as an attractive candidate for applications in quantum information science. Due to their ability to create well localized states within the band gap, these deep defect levels can serve as isolated atoms which can be utilized as single photon emitters (SPE) and defect-based qubits. Engineering point defects in 2D materials gives the advantage of reduced dielectric loss and the possibility of integrating with waveguides and cavities. First-principles calculations have been effective in complementing and validating experiments by identifying potential defect species and characterizing their optical response. One key ingredient that can be obtained at the density functional theory (DFT) level is the defect formation energy, which is the energy penalty of creating a defect in the pristine crystal. The formation energy can then be used to determine the equilibrium concentration of all possible defect species to occur in a specific crystal. Studying defect emission and excited-state dynamics in general requires methods beyond DFT such as time-dependent (TD-) DFT, but it is often possible to approximate the excited states by manipulating level occupancies by the so called ΔSCF method at the DFT level. These methods allow us to investigate optical transitions and electron-phonon coupling and compare these results to experimentally measured transition energies and Huang-Rhys factors. In our work, we study neutral and charged defects in monolayer hexagonal boron nitride (h-BN), using boron and nitrogen vacancies as prototypical examples. Formation energies, optical transition levels, relaxation energies, and the Huang-Rhys factors were obtained in the one-dimensional configuration coordinate diagram (1D-CCD) approximation, where the atomic displacements can be simplified into one collective coordinate. These results are to be compared to phonon spectra calculations. Ultimately, the goal is to access the validity of the 1D-CCD approximation for its potential use in high-throughput screening, and to identify defects that serve as ideal candidates for single phonon emitters, which requires deep defect levels and small electron-phonon coupling.