Designing Point Defects with Low Electron-Phonon Coupling in 2D Materials

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Point defects in semiconductors are promising for quantum information science applications due to their ability to form well-localized states within the band gap, acting as isolated atoms that can be utilized as single photon emitters (SPEs) and spin qubits. A key factor for higher photon indistinguishability, essential for effective SPEs, is small electron-phonon coupling, often measured by Huang-Rhys (HR) factors. Calculating HR factors is complex, and their numerical values are typically used without establishing a meaningful link to the physical defect system. Identifying this link could guide the design of defects to minimize HR factors.

We propose that small HR factors correspond to the preservation of bonding-character between the initial (occupied) and final (unoccupied) states in a transition. We demonstrate this for realistic SPE candidates in hBN defect systems and diamond NV centers. HR factors are calculated using first-principles within the one-dimensional configuration coordinate diagram (1DCCD) approximation and compared with full phonon spectra calculations. These calculations involve extrapolating spectral functions towards the dilute defect limit using an embedding method that relies on the limited range of interatomic force constants in covalent semiconductors. The calculated HR factors are then correlated with the bonding-character similarity between the excited and ground states.