Visible Transition in Localized Defect-mediated h-BN Monolayer  

SHENG YU, TIKARAM NEUPANE, BAGHER TABIBI, FELIX JAETAE SEO, Hampton University — The studies of spin-resolved electronic bandstructure and electron density of states (DoS) for the defect-mediated hexagonal boron nitride (h-BN, \(E_B \approx 5.2 \text{ eV}\)) monolayer revealed the formation of energy states within the forbidden band and the electron spin-dependent optical transitions between the energy states in visible spectral region. The absorption and reflection coefficients of defect-mediated h-BN were analyzed by the density function theory (DFT). The localized point defects in h-BN included boron vacancy (\(V_B\)), nitrogen vacancy (\(V_N\)), boron replacing nitrogen (\(B_N\)), nitrogen replacing boron (\(N_B\)), carbon replacing boron (\(C_B\)), carbon replacing nitrogen (\(C_N\)), boron replacing nitrogen with boron vacancy (\(B_N-V_B\)) and nitrogen replacing boron with nitrogen vacancy (\(N_B-V_N\)). The prospective nonlocal correlation between electron spin and photon polarization in the defect-mediated h-BN will pave the application of quantum information processing with two-dimensional atomic layer solid-states.

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