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Visible
Transition in Localized Defect-mediated h-BN Monolayer[1] 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~5.2 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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