**Computational quantum information materials**

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Optically addressable spin defects in wide-gap semiconductors have recently shown immense promise for use in solid-state quantum applications owing to their robust spin properties, high fidelity spin-to-photon conversion, and high-temperature functionality[1]. Furthermore, several vacancy defects in SiC have featured prominently in the search of new and improved solid-state qubits compatible with wafer-scale device fabrications and telecommunication technologies[2]. Consequently, a significant interest has emerged to discover novel defect-based qubits in much more diverse materials systems for broadening the scope of the solid-state quantum information[3]. In this study, we highlight some of our recent efforts devoted to first-principles computational design of new spin defects in hexagonal boron nitride (h-BN). h-BN has been recently found to host a variety of single-photon emitters[4]. However, optically addressable spin qubits, such as the diamond NV center, have not yet been realized in h-BN. In this talk, we discuss carbon dimer defects as promising candidates of optically active spin qubits in h-BN [5]. We use first-principles hybrid density functional theory and quantum embedding theory to investigate its structural and electronic properties. We show that the C2 defect features a 3A2 spin-triplet ground state, arising from defect-induced deep levels in the band gap of the host material, and localized unpaired electrons. We calculate the optical zero phonon line of the defect’s spin-conserving 3A2 - 3E excitation to be 2.1 eV. By comparing the defect formation energy of the C2 defect and other C-related defects, we show that the C2 defect is energetically stable in h-BN. Our study aimed at searching new coherent spin qubits is a significant step towards the realization of individually addressable spin qubits in two-dimensional hexagonal boron nitride.

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