First-principles theory of defect-based quantum bits in semiconductors

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In recent years, remarkable advances have been achieved in the development of defect-based spin quantum bits (qubits) in semiconductors for solid-state quantum information science and technology. Promising spin qubits include the nitrogen-vacancy center in diamond, dopants in silicon, and the silicon vacancy and divacancy spins in silicon carbide. In this talk, I will highlight some of our recent efforts devoted to defect spin qubits in functional wide-gap semiconductors [1-6]. In the first part of the talk, I will explain basic concepts of using point defects in semiconductors as qubits and their quantum applications. Then, I will describe our recent result on first-principles computational design of new spin defects for use as qubits in piezoelectric crystals such as AlN and SiC. I will also discuss opportunities and recent results on quantum defects found in 2-dimensional van der Waals materials systems. In particular, I will present our recent combined experimental and theoretical study on Stark tuning of single photon emitters in h-BN/graphene heterostructure [1] and also a theoretical study on quantum decoherence in 2-dimensional worlds [2]. I will conclude my talk by discussing a perspective of combining density functional theory [3] and cluster correlation expansion calculations [4] to predict not only the thermodynamic and electronic properties of defect qubits, but their coherent quantum properties from first-principles.

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