Solid-state quantum information science using defects in semiconductors

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In recent years, remarkable advances have been reported in the development of defect 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 wide-gap semiconductors [1-4]. In the first part of the talk, I will explain basic concepts of using point defects in semiconductors as qubits and their applications. Then, I will describe our recent combined theoretical and experimental study on remarkably robust quantum coherence found in the divancancy qubits in silicon carbide [2]. We used a quantum bath model combined with a cluster expansion method to identify the microscopic mechanisms behind the unusually long coherence times of the divacancy spins in SiC. I will also discuss progress and challenges in computational design of new spin defects for use as qubits in piezoelectric crystals such as AlN and SiC, including a new defect design concept using large metal ion - vacancy complexes [1]. Our first principles calculations include DFT computations using recently developed self-consistent hybrid density functional theory and large-scale many-body GW theory.

[1] H. Seo, H. Ma, M. Govoni, and G. Galli, *submitted* (2017).

[2] H. Seo, A. L. Falk, P. V. Klimov, K. C. Miao, G. Galli, and D. D. Awschalom, Nature Communications **7**, 12935 (2016).

[3] H. Seo, M. Govoni, and G. Galli, Scientific Reports **6**, 20803 (2016).

[4] W. F. Koehl, H. Seo, G. Galli and D. D. Awschalom, MRS Bulletin **40**, 1146 (2015).