MAR17-2016-020266

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Simulations of defect spin qubits in piezoelectric semiconductors[1]

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In recent years, remarkable advances have been reported in the development of defect spin qubits in semiconductors for solid-state quantum information science and quantum metrology. 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 piezoelectric wide-gap semiconductors for potential applications in mechanical hybrid quantum systems [1-3]. In particular, I will describe our recent combined theoretical and experimental study on remarkably robust quantum coherence found in the divancancy qubits in silicon carbide. 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. Our study indicates that developing spin qubits in complex crystals with multiple types of atom is a promising route to realize strongly coherent hybrid quantum systems. 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. 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, A. L. Falk, P. V. Klimov, K. C. Miao, G. Galli, and D. D. Awschalom, Nature Communications 7, 12935 (2016). [2] H. Seo, M. Govoni, and G. Galli, Scientific Reports 6, 20803 (2016). [3] W. F. Koehl, H. Seo, G. Galli and D. D. Awschalom, MRS Bulletin 40, 1146 (2015).

[1]This work was supported by the National Science Foundation (NSF) through the University of Chicago MRSEC under award number DMR-1420709.