Defects in semiconductors for quantum information science

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Introduction

Deep-level defects in wide-bandgap semiconductors exhibit localized electronic energy levels with paramagnetic spin states, and hence they constitute promising platforms for quantum bits (qubits).

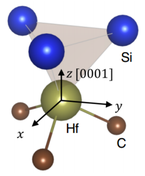
Using density functional theory (DFT) with dielectric hybrid functionals[1,2] and many-body perturbation theory[3,4] implemented in the WEST code, we predicted the electronic structures of deep-level defects in semiconductors. Utilizing parameters extracted from DFT, we built spin Hamitonian that we then used to compute spin-spin correlation times T_2.

Electronic structure prediction of novel defects as promising qubit candidates

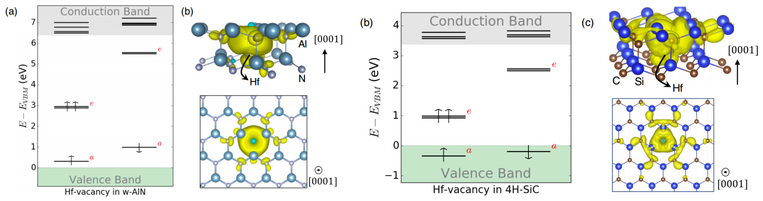
Large transition metal ion-vacancy complexes in 4H-SiC and AlN[5]

Based on DFT calculations, we proposed that large transition metal ion (La, Hf, Y)-vacancy complexes in 4H-SiC and AlN have promising properties as spin qubits:

- Stable triplet spin states in the band gap.
- Optically addressable defects (~2eV zero phonon line).
- Significant coupling to the lattice through silicon dangling bonds, facilitating mechanical manipulation of spin states.



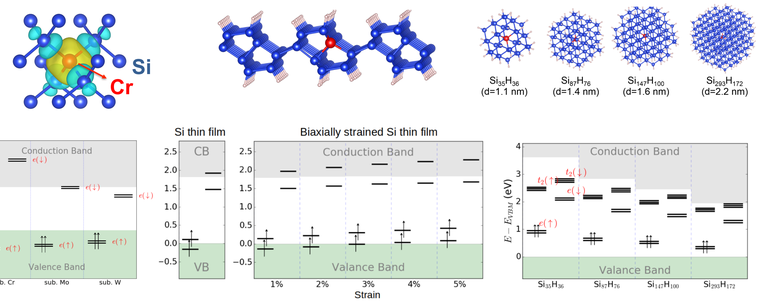
Defect levels and spin densities:



Group-6 transition metal ion impurities in silicon[6]

Using DFT calculations, we found that group-6 transition metal ion impurities (Cr, Mo, W) are promising spin qubits in low dimensional silicon:

- Stable triplet spin states with localized spin density have been identified.
- In strained silicon films and silicon nanoparticles, spins are carried by symmetry-protected levels located in the band gap.



Optical addressability is a critical property to design spin qubits. We are developing a method based on the solution of the Bethe-Salpeter equation to predict the optical excitation spectra of defects in semiconductors and insulators[7,8].

Prediction of spin Hamiltonian parameters for defects

The spin Hamiltonian of a spin qubit **S** in a nuclear spin (**I**) bath with an external magnetic field **B** is:

$$H = H_S + H_B + H_{int}$$

$$H_S = \beta \mathbf{S}\cdot\mathbf{g}\cdot\mathbf{B} + \mathbf{S}\cdot\mathbf{D}\cdot\mathbf{S}, \quad H_B = -\mathbf{B}\cdot\sum_i \gamma_i \mathbf{I}_i + H_{n-n}, \quad H_{int} = \mathbf{S}\cdot\sum_i \mathbf{A}_i\cdot\mathbf{I}_i$$

$$H_{n-n} = \frac{\mu_0}{4\pi}\sum_{i<j}\gamma_i\gamma_j\hbar^2\left(\frac{\mathbf{I}_i\cdot\mathbf{I}_j}{r_{ij}^3} - \frac{3(\mathbf{I}_i\cdot\mathbf{r}_{ij})(\mathbf{I}_j\cdot\mathbf{r}_{ij})}{r_{ij}^5}\right)$$

- Hyperfine interaction **A** contributes to spin decoherence.
- Zero field splitting **D** determines the energy gap between spin sublevels.
- We are developing finite element based methods to accurately predict **A**, **D** and the **g** tensor from first principles[9].

Quantum decoherence of spin qubit

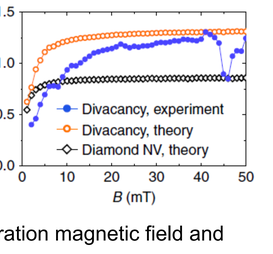
Long coherence is key to the performance of qubits. The phase coherence time T_2 of solid-state spin qubits is intrinsically limited by the nuclear spin bath.

Time evolution of the spin density matrix

$$\rho_{tot}(t) = \mathcal{U}(t)\rho_{tot}(0)\mathcal{U}^{\dagger}(t)$$

Coherence function $\mathcal{L}(t) \equiv \frac{tr[\rho_{tot}(t)S_+]}{tr[\rho_{tot}(0)S_+]}$

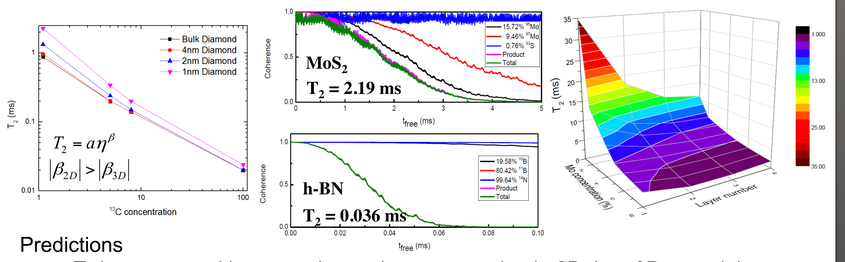
The coherence function L(t) is computed using the cluster-correlation-expansion method.



Decoherence of divacancy spin in SiC[10]

We accurately predicted the T_2 of divacancy in SiC at saturation magnetic field and explained why the T_2 is longer in SiC than in diamond.

Decoherence in two-dimensional materials[11]

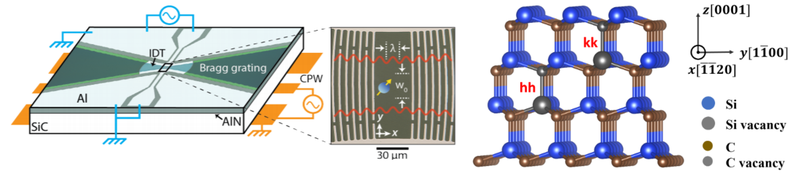


Predictions

- T_2 is more sensitive to nuclear spin concentration in 2D than 3D materials.
- T_2 enhancement for 2D materials is stronger at low concentrations.
- MoS_2 is a promising host material for spin qubit.

Mechanical driving of defect spins

Divacancies in 4H-SiC are prototypical spin qubits and they can be manipulated by surface acoustic waves (SAW). We performed theoretical studies to understand the magnitude of the coupling between spin and acoustic waves and to investigate how the coupling is influenced by the crystal symmetry of 4H-SiC.[12]

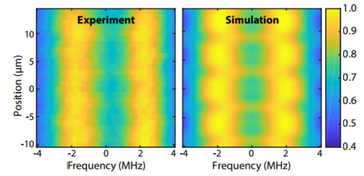


The resonance energy between different spin states is characterized by the zero-field-splitting tensor **D**, which is coupled to the lattice strain **ε** through the spin-strain coupling tensor **G**:

$$G_{ij} = \frac{\partial D_i}{\partial \varepsilon_j}$$

We predicted the value for the spin-strain coupling tensor **G** by DFT calculations.

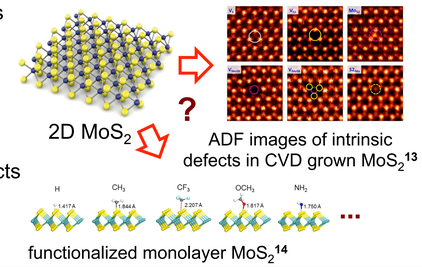
We reproduced the zero-field splitting as a function of longitudinal ([-1-120] direction) position in a Gaussian SAW resonator.



Identification of novel defects in 2D materials

2D materials are promising host materials for defects with novel spin and electronic properties, and sophisticated synthesis methods are emerging to fabricate such systems, in particular 2D transition metal dichalcodenides.

Work is in progress to identify novel defects in 2D MoS_2 ranging from intrinsic vacancies, and dopants to functional groups.



References and Acknowledgements

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