



HARVARD Quantum Optics Center

Special Quantum Sciences Seminar

Thursday | Mar. 6 | 3:00 pm
Jefferson 356*

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" Quantum Mechanical Simulations of Solid State Quantum Bits "

Nitrogen-vacancy center in diamond has become a leading quantum measurement solid state device. Understanding the intricate details of its electronic structure, magnetic and optical properties, the process of non-radiative decay from the excited state as a function of external perturbation or temperature is inevitable in order to optimize its operation. Particularly, we show that advanced density functional theory is able to address this issue. Our recent developments on calculating the electron spin - electron spin dipole-dipole interaction can provide insight about the effect of perturbations on NV-center. The measurement of these external perturbations may be utilized for sensing quantum objects such as single electron or nuclear spins. However, many materials science problems have to be solved in practice. Our calculations indicate that the formation of NV defect in electron irradiated or N-implanted diamond samples occurs in the early stage, and optically active, high-spin divacancy defects form in this process. We also show that there is a critical distance between the position of NV defect and the surface of diamond to preserve their favorable properties found in bulk diamond, and we identify such combination of terminators at (001) surface of diamond, which would be ideal for sensing applications.

Refreshments will be served at 2:50 PM.

*Please note the day, location, and time change