

Modeling next-generation quantum emitters and sensors

Motivation:

After a century of research, technologies that directly harness quantum effects are now becoming viable. However, within the realm of quantum information, sensing, and metrology, significant needs exist for the design and characterization of materials having characteristics that allow for quantum technological applications. The ensuing knowledge gap underscores a need for more modeling of theoretical defect sites in diamond, silicon carbide, and related materials, to identify potential candidates for experimental investigation.

Background:

Quantum technologies demand unique materials properties which depend on the specific application. For example, key properties of materials for quantum information processing include single photon sources that are photostable, work at room temperature, evidence a strong zero phonon line, and have short excited state lifetimes [1]. Quantum metrological applications rely on factors such as fine structures that are dependent on strain and electric / magnetic field interactions, optical spin-polarization effects, and ground state electronic spins with long coherence times [2].

Single photon sources have been identified in systems such as diamond, silicon carbide, and hexagonal boron nitride. Out of the hundreds of known color centers in diamond, relatively few are single photon emitters, and most emitters emit in the visible or near infrared bands [1,3]. To eliminate the need for costly infrastructure buildout, a single photon source that operates within current telecommunications channels (i.e. 1550 nm) would represent a significant advancement. The nitrogen-vacancy (NV) center in diamond has been studied as a single photon source, but the existence of a significant phonon sideband compromises the photon generation efficiency. The NV center has also been studied in the context of quantum sensing and metrological applications, where applications to date include nanoscale magnetometry, electrometry, and biosensing [2]. This challenge acknowledges that other color centers may have material properties that are more favorable than known systems for high rep-rate single photon sources, quantum sensing, and metrology. The rapid identification of such color centers and prediction of their photophysical properties would impact the existing quantum technology industry [4].

Project Details:

The goal of this project is to guide color center engineering efforts by performing theoretical studies of defect sites of interest for quantum technologies. Defects of interest include transition metal color centers in diamond, SiC, or GaN [5,6]. Student teams will theoretically model defect sites of interest with respect to physical parameters key to quantum technological applications. Factors of interest include: absorption energy, emission wavelength, excited state lifetime, and the dependence of these quantities on electric, magnetic, and strain fields. Bulk or nanoparticle morphologies may be considered. Given the complexity of the research involved, student teams should leverage existing work that has developed cluster geometries and identified optimal density functionals for specific defect sites [5-6], and focus their efforts narrowly on determining

one or two key parameters that are of interest. The results of this research will be tested within AFRL/RXAN, using our facilities for color center synthesis and characterization.

Expectations:

The proposer must have access to a high performance computing cluster or the ability to access time on such a cluster. The sponsor has available hours on servers within the AFRL High Performance Computing Center, but a locally available cluster will enhance the likelihood of a successful project. This work will likely involve a ~1 year effort. Ideally the team would host a visit by the sponsor or designee during the fall. A final presentation may be given onsite or at the host institution. A successful proposal should outline which defect sites will be investigated, the projected methodology and level of theory, and identify expected deliverables. For example, the emission wavelength or dependence of the emission wavelength on magnetic field for a defect or series of defects could be calculated. Appropriate methods include using time-dependent density functional theory in either computational clusters or supercells with periodic boundary conditions. In framing the proposal, consideration should be given to specific technological applications.

Skills Needed:

- 1) Understand and run public-license computational software packages (e.g., GAMESS, NWChem, Quantum Espresso)
- 2) Familiarity with Linux/Unix OS
- 3) Completion of or enrollment in an introductory quantum mechanics course

Sponsor

Air Force Research Laboratory – Materials & Manufacturing Directorate, WPAFB, OH
Nanoelectronics Branch, RXAN

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References

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2. Doherty, M. W. *et al.* The nitrogen-vacancy colour centre in diamond. *Physics Reports* **528**, 1 (2013).
3. Gaebel, T. *et al.* Stable single-photon source in the near infrared. *New J. Phys.* **6**, 98 (2004).
4. See, e.g., <http://quantumdiamondtech.com/> and <http://quandela.com/>.
5. N. W. Gothard, *et al.* Modeling of transition metal color centers in diamond. *MRS Advances FirstView*, 1–5 (2016).
6. W. F. Koehl, *et al.* Resonant optical spectroscopy and coherent control of Cr⁴⁺ spin ensembles in SiC and GaN. *Phys. Rev. B* **95**, (2017).