The Ups and Downs of Quantum Sensing: exploring the feasibility of exploiting spin-polarised states in TiO_2

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While the manipulation of shallow point defects in bulk crystal semiconductors was foundational to the digital age, it is exploitation of their deep-level counterparts that has beckoned in the quantum age [1]. When deep-level point defects in wide-bandgap materials form highly spatially localized, atom-like spin states which are vibronically decoupled from the host crystal, they can function as single solid-state spin systems and fulfil the DiVincenzo criteria for quantum computation [2]. Quantum sensing, based on solid-state spin systems, is a rapidly advancing field that holds immense potential for a wide range of applications, from medical diagnostics to national security [3]. While the use of nitrogen-vacancy (NV^-) centers in diamond has been a prominent approach, there are limitations, such as the inability to fashion the diamond host into high precision cantilevers required for scanning probes, that have driven the exploration of alternative materials. Recent key advances in facile synthesis methods of TiO_2 quantum dots and nanocrystals of controlled oxygen vacancy concentrations [4] and titanium [5] offer the ability to tailor the concentration of spin-polarized defect states. Compared to other quantum sensing material candidates, TiO_2 offers several advantages. It is abundant, cost-effective, environmentally friendly and malleable to form high precision scanning probe tips. Additionally, TiO_2 can be easily integrated into existing semiconductor manufacturing processes, making it a promising candidate for scalable quantum sensing technologies.

In this work, we explore the feasibility of utilizing ferromagnetic semiconductor TiO_2 quantum dots and nanocrystals as contender material systems for the next generation of quantum sensors. The intriguing room temperature ferromagnetic behavior of nonmagnetic oxides has been attributed to intrinsic defect-induced spin-split states [6]. We examine the propensity to form deep-level atom-like spin-states in the TiO_2 anatase wide optical bandgap. We employ inverse modeling of reported experimental data [5] to constrain the parameter space to predict ground-state point defect geometries for viable solid-state spin qubits.

References

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