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Spin-Active Defects in Layered Hexagonal BeO: A Wide-Bandgap 2D Host for Quantum Technologies

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Precise control of quantum states is a key requirement for the development of quantum-based technologies. Engineering point defects in low-dimensional materials provides a promising approach to achieving this control, as strong in-plane coupling can accelerate quantum gate operations while mitigating decoherence. Hexagonally layered beryllium oxide (h-BeO) is a recently synthesised two-dimensional material with a wide bandgap, offering the potential to host highly localised defect states suitable for qubit implementation and quantum sensing.

In this study, we employ density functional theory to investigate the structural and electronic properties of ultra-thin and bulk h-BeO and to evaluate the feasibility of defect-based qubits. We identify several point defects exhibiting non-zero ground-state spins and optically addressable transitions. The calculated defect levels and transition energies indicate that h-BeO can provide stable, well-isolated spin states within its bandgap, enabling coherent control and optical readout.

Our results position h-BeO as an interesting platform for defect-based quantum technologies, expanding the range of viable two-dimensional hosts for qubits. This work advances the understanding of native defect physics in wide-bandgap oxide-based layered materials, bridging the gap between theoretical prediction and experimental realisation.

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