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Accurate hyperfine tensors for electrons and holes in Si and GaAs

PERICLES PHILIPPOPOULOS, McGill University, STEFANO CHESI, Beijing Computational Science Research Center, WILLIAM COISH, McGill University — Knowing (and controlling) hyperfine interactions in semiconductor nanostructures is important for quantum information processing with electron, hole, and nuclear-spin states. Through a combination of first-principles density-functional theory calculations and $\mathbf{k} \cdot \mathbf{p}$ corrections, we have found accurate hyperfine tensors for electrons and holes in GaAs and Si. Our results indicate significant corrections to previous theoretical estimates for the hyperfine coupling of electrons in GaAs and Si, but are consistent with earlier experimental measurements on Knight shifts and Korringa relaxation. In addition, we make new predictions for the hyperfine tensors of both heavy and light holes in the valence band. These calculations are consistent with T_2^* times very recently measured for heavy holes in Si quantum dots [1], and with recent measurements on hole spins in InGaAs quantum dots showing an Ising-like hyperfine coupling [2]. [1] Maurand et al., arXiv:1605.07599 (2016). [2] Prechtel et al., Nat. Mat. 15, 981 (2016).

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