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First-principles hyperfine tensors for electrons and holes in silicon and GaAs PERICLES PHILIPPOPOULOS, McGill University, STEFANO CHESI, Beijing Computational Science Research Center, WILLIAM COISH, McGill University — Knowing (and controlling) hyperfine interactions in silicon and III-V semiconductor nanostructures is important for quantum information processing with electron and nuclear spin states. We have performed density-functional theory (DFT) calculations that fully account for spin structure of the Bloch states (in contast with approaches that rely on the density alone). Using this method, we confirm the known value for the contact hyperfine coupling in the conduction band of silicon, but find a significant deviation in the value for the conduction band of GaAs relative to the accepted value, estimated in ref. [1]. Moreover, this method can be used to calculate the full hyperfine tensor for the valence band, where spin-orbit effects may be strong, precluding methods that determine hyperfine couplings from the density alone. This general method can be applied to a broad class of materials with strong combined spin-orbit and hyperfine interactions. [1] D. Paget, G. Lampel, B. Sapoval, and V. I. Safarov Phys. Rev. B 15, 5780 (1977)

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