Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Ab-initio calculation of spin relaxation times OSCAR D. RE-STREPO, WOLFGANG WINDL, The Ohio State University — One of the most fundamental questions in spintronics to date concerns the ultimate limit of spin relaxation times. We have been developing for the first time a parameter-free first-principles method to determine spin relaxation times. Our effort initially concentrates on silicon and diamond. For liquid-nitrogen temperatures and above, spin relaxation in silicon is dominated by the Elliott-Yafet mechanism. The spin relaxation is induced by momentum scattering off impurities or phonons. The development of a basic methodology based on density-functional calculations that can be used to determine momentum scattering lifetimes has been recently completed by one of us [1]. By considering the spin-orbit mixing of the up and down states, the spin-flip matrix elements can be related to the momentum matrix elements. The underlying theory has previously been derived for III-V semiconductors with direct band gap but did previously not exist for indirect-band gap materials such as silicon or diamond. We report results of an accurate formulation to calculate spin relaxation times in silicon and diamond based on first-principles methods, which we find in excellent agreement with experimental relaxation times. Due to the ab-initio nature of our method, it can be directly applied to study other potentially spin-preserving systems.

[1] O. D. Restrepo et al., Appl. Phys. Lett. **94**, 212103 (2009).

oscar restrepo
The Ohio State University

Date submitted: 28 Nov 2009   Electronic form version 1.4