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Non-perturbative ab-initio calculation of the g-tensor in periodic boundary conditions

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Electron Paramagnetic Resonance (EPR) spectroscopy is one of the most powerful and versatile analytic tools in materials science to date. The wealth of important information available from EPR spectroscopy, however, cannot be extracted from experiments alone, rather from the combination of experimental data and theoretical calculations. To date, first principle methods for computing the EPR g-tensor rely on the linearization of the effective spin Hamiltonian with respect to spin orbit (SO) coupling [1]. While this approach gives good results for light atoms, it is insufficient when SO coupling is strong, as in transition metal compounds. We have derived a method to calculate the electronic g-tensor of paramagnetic defects from first principles in a non-perturbative way, based on the formula for the orbital magnetization [2]. The main advantage of this method, is that the external magnetic field does not enter the formula explicitly, showing that the g-tensor can be calculated as a ground state quantity by including the spin-orbit term in the SCF hamiltonian. We have found a perfect agreement with linear response calculations for bulk systems and molecular complexes containing light atoms. For heavier atoms, the agreement with experimental data is substantially improved.

[1] C. J. Pickard and F. Mauri, Phys. Rev. Lett. 88, 086403 (2002).

[2] D. Ceresoli, T. Thonhauser, D. Vanderbilt and R. Resta, Phys. Rev. B 74, 024408 (2006); D. Xiao, G. Vignale, J. Shi and Q. Niu, Phys. Rev. Lett. 99, 197202 (2007).