

All-electron magnetic response with pseudopotentials: NMR chemical shifts

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We present a theory for the *ab initio* calculation of all-electron magnetic response in insulators with pseudopotentials [1]. So far, derivations of pseudopotential Hamiltonians have not dealt with magnetic fields. To correctly describe the interaction between orbital degrees of freedom and magnetic fields within a pseudopotential approach, we introduce an extension of Blöchl's Projector Augmented-Wave (PAW) method, that we call the Gauge Including Projector Augmented-Wave (GIPAW) approach. Contrary to the original PAW formalism, the GIPAW method is invariant upon translation in presence of a constant magnetic field. Using GIPAW i) we derive a pseudo-Hamiltonian in presence of a constant magnetic field, ii) we compute the linear perturbation of pseudo-wavefunctions with respect to a constant magnetic field, iii) we reconstruct the induced all-electron current from the perturbed pseudo-wavefunctions. Finally, the knowledge of the induced all-electron current allows us to compute the induced magnetic field at the nuclear positions, which defines the NMR chemical shifts. We successfully validate our theory by comparison with all-electron results for molecules and solids.

[1] C. J. Pickard, F. Mauri, Phys. Rev. **B 63**, 245101 (2001).