O.20 Orbital magnetism in the projector-augmented wave formalism

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We show how to compute the first-order change of the energy due to an homogeneous magnetic field, within the projector-augmented wave formalism of density functional theory, for an insulator with periodic boundary conditions. To accomplish this we use a perturbative treatment of the density operator, in which magnetic translation symmetry is invoked in order to obtain well-posed expressions, and which generalizes the modern theory of orbital magnetization. Further, we observe that the gauge invariance of the resulting terms permit the use of density functional perturbation theory to compute the necessary wavefunction derivatives, rather than the finite difference approach that has been used previously. In order to obtain nontrivial magnetization, we also impose nuclear magnetic dipole moments on atomic sites of interest. The resulting expressions have been implemented and tested, and results are shown both for an atomic test case and for a variety of solids, for which the chemical shielding as measured in nuclear magnetic resonance experiments is obtained.