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**Projector Augmented-Wave formulation of response to strain and electric field perturbation within the density-functional perturbation theory** ALEXANDRE MARTIN, CEA-DIF, Arpajon, France, MARC TORRENT, CEA-DIF, Arpajon, France, RAZVAN CARACAS, CNRS - ENS Lyon, France — A formulation of the response of a system to strain and electric field perturbations in the pseudopotential-based density functional perturbation theory (DFPT) has been proposed by D.R Hamman and co-workers. It uses an elegant formalism based on the expression of DFT total energy in reduced coordinates, the key quantity being the metric tensor and its first and second derivatives [1]. We propose to extend this formulation to the Projector Augmented-Wave approach (PAW). In this context, we express the full elastic tensor including the clamped-atom tensor, the atomic-relaxation contributions (internal stresses) and the response to electric field change (piezoelectric tensor and effective charges). With this we are able to compute the elastic tensor for all materials (metals and insulators) within a fully analytical formulation. The comparison with finite differences calculations on simple systems shows an excellent agreement. This formalism has been implemented in the plane-wave based DFT ABINIT code. We apply it to the computation of elastic properties and seismic-wave velocities of iron with impurity elements. By analogy with the materials contained in meteorites, tested impurities are light elements (H, O, C, S, Si).

[1] D.R Hamman et al., Phys. Rev. B 71, 035117 (2005)

Marc Torrent
CEA-DIF

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