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Ab-initio computation of Raman spectra within the DFPT-PAW formalism LUCAS BAGUET, MARC TORRENT, CEA DAM DIF — The interpretation of experimental Raman spectra of materials is, in general, a difficult task. To compare these spectra with theoretical ones gives a deeper understanding of the underlying physics phenomena. The computation of theoretical Raman spectra require the third-order derivatives of the ground state energy, which can be done using the $2n + 1$ theorem, as in the Density Functional Perturbation Theory (DFPT), or with finite difference methods. Existing works using the $2n + 1$ theorem are limited to norm-conserving (NC) (as in Veithen *et al*, Phys. Rev. B 71, 125107 (2005)) or ultra-soft (US) pseudo-potentials (Miwa, Phys. Rev. B 84, 094304 (2011)). We present a method adapted to the projector-augmented wave (PAW) formalism, which conciliate the small cost of NC pseudo-potentials with the precision of all-electron calculations. Contrary to Veithen *et al*, the electric field perturbation is treated analytically, leading to the resolution of a second-order Sternheimer equation (as in the work of Miwa). Comparing the different approaches, our results show that the analytical one has the best k-point convergence.

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