Ab-initio computation of Raman spectra within the DFPT+PAW(+U) formalism

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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 physical phenomena. Using Density-Functional Perturbation Theory, phonon modes are obtained at the second order of perturbation, giving the peak positions.
Raman intensities are computed from a third order perturbation with respect to an atomic displacement and the application of an electric field [1, 2].
Several implementations of Raman intensities exist, but they are limited to norm-conserving [1, 2], or ultra-soft pseudo-potentials [3]. Recently, Raman intensities have been obtained in DFT+U [4], which is more precise for correlated materials. Here, we present the new Abinit implementation valid for norm conserving and PAW pseudo-potentials. After a little reformulation of the PAW+U method [5], DFPT+PAW computations, including the third order, can include "+U" terms without too much implementation work.
Finally, we present how Raman intensities are computed in practice and discuss the comparison of theoretical spectra with experimental ones.

References

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