

Ab-initio calculation of vibrational Raman spectra in large systems

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I will present an approach [1] for the efficient calculation of vibrational Raman intensities in periodic systems within density functional theory. The Raman intensities are computed from the second order derivative of the electronic density matrix with respect to a uniform electric field. In contrast to previous approaches, the computational effort required by our method for the evaluation of the intensities is negligible compared to that required for the calculation of vibrational frequencies. As a first application, we study the signature of 3- and 4-membered rings in the the Raman spectra of several polymorphs of SiO₂, including a zeolite having 102 atoms per unit cell.

[1] M. Lazzeri and F. Mauri, Phys. Rev. Lett., accepted for publication.