Exploring the microscopic structure of minerals through *ab initio* vibrational spectroscopy

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Ab initio electronic structure calculations are nowadays a mature tool to predict the lattice dynamics of condensed phase systems, such as minerals [1]. Besides the full set of vibrational frequencies, accurate infra-red (IR) and Raman spectra can be computed, enabling a direct and synergistic comparison with the experiments [2-4].

Simulation allows the investigation of the effect on vibrational spectra due to variables such as chemistry, composition, isotopic content, disorder, polymorphism, and microsopic structure, going beyond the limits imposed by natural samples and experimental set-ups. Relationships can be readily established, between these factors and the observed spectral features.

This presentation will discuss how simulated IR and Raman spectroscopies can be used to investigate structural aspects in disordered minerals, with particular focus on substitutional [5] and orientational disorder [6].

[1] Dovesi *et al*. (2011) *Am. Mineral*. **96**, 1787-1798. [2] De La Pierre *et al*. (2013) *J. Comput. Chem*. **34**, 1476-1485. [3] Carteret *et al*. (2013) *J. Chem. Phys*. **138**, 014201. [4] De La Pierre *et al*. (2014) *J. Chem. Phys*. **140**, 164509. [5] De La Pierre *et al*. (2013) *Am. Mineral*. **98**, 966-976. [6] De La Pierre *et al*. (2014) *J. Phys. Chem. C* **118**, 27493-27501.