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Ab-initio vibrational properties of minerals

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Ab-initio computational methods based on the density functional theory (DFT) can nowadays accurately reproduce the structure and the electronic properties of a wide variety of materials and systems: isolated molecules, crystals, amorphous systems, liquids, surfaces etc. Moreover, the use of sophisticated techniques such as DFT linear response allow the determination of vibrational properties and thus of phonon dispersions, dielectric constants, infrared and Raman spectra. Thank to the possibility of a precise description at the microscopic level of so many phoenomena, the ab-initio methods have become nowadays an almost essential instrument for the correct interpretation of several experimental results. In this talk I will show examples of the possibilities given by the ab-initio approach, and applications of our recently-developed method to determine vibrational Raman spectra. In particular, I will talk about the determination of the signature of small-rings defects in SiO2 polymorphs, and our study of the OH-stretching modes in kaolinite group minerals.