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Phonon Raman scattering from first principles

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Light propagating through a crystal can be inelastically scattered by lattice vibrations. Thereby the exciting light beam experiences a frequency shift which is detected in the Raman experiment. This *Raman shift* is caused by the modulation of the material's polarizability upon time-dependent ionic displacements. Experimental Raman data thus contain a wealth of information about phonons, electronic structure, as well as their interplay. For instance, temperature-dependent lineshapes and overtone spectra can be related to the extent of anharmonic effects, and strong electron-phonon interaction is expressed in terms of large scattering intensities. The assignment of frequencies to specific vibrations typically relies on comparison with reference systems by considering atomic masses and the symmetry of the crystal. For an in-depth understanding of the measured features and an unambiguous assignment of modes, *ab initio* theory can provide valuable insight. In the Raman spectra, the peak positions correspond to the phonon frequencies and thus can be solely determined from frozen-phonon or linear-response calculations. The scattering intensities, however, involve the change of the frequency-dependent complex dielectric tensor with atomic displacements along the phonon eigenvector. All these quantities can be obtained from density-functional theory (DFT) in combination with time-dependent DFT or many-body perturbation theory. In this talk, I will review how to compute Raman spectra from first principles. Selected examples will demonstrate the effects of isotope substitution, anharmonicity, temperature, and excitation energy, as well as the role of symmetry. They reveal that Raman scattering is a beautiful technique as it reflects basic principles of quantum mechanics as much as complex excitations of complex matter.