Crystal Structure Prediction with WIEN2k

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The ground state properties of solids are calculated within density functional theory (DFT) using the WIEN2k code [1] that is based on the full-potential augmented plane wave (APW) method. From the total energy the relative stability of different structures can be compared. By minimizing the forces acting on the atoms we can optimize the atomic positions. For the relaxed geometry the electronic structure is known, from which properties and spectra can be calculated. Phonons can be obtained with a direct method, in which the dynamical matrix is derived from a set of forces that are created when a single atom is displaced along a symmetry-adapted direction in a supercell containing 60-100 atoms. From a limited number of such displacements the complete phonon spectrum can be derived.

Such calculations will be illustrated for $Y_2Nb_2O_7$ that (based on powder diffraction) was proposed to crystallize in the pyrochlore structure and experimentally was found to be an insulator [2]. DFT calculations would make it metallic but the phonons indicate an instability that leads to a significant distortion of the structure, in which it is an insulator. Another example is the ferroelectric phase transition that occurs in the Aurivillius compound $SrBi_2Ta_2O_9$. In this case three phonons, a combination of 1 hard and 2 soft phonon modes, are needed to describe this unconventional ferroelectric phase transition.

[1] Schwarz K., Blaha P., Madsen G.H.K., *Comp. Phys. Commun.*, 2002, **147**, 71. [2] Blaha P., Singh D.J., Schwarz K., *Phys. Rev. Lett.*, 2004, **93**, 216403.

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