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Identifying minerals based on the WURM database

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Abstract

The WURM project aims [1] to build a freely accessible web-based database of computed physical properties for minerals and ices. The database provides for each mineral various physical properties: the crystal structure used in the calculation, the dynamical charges and the dielectric tensors, the refractive index, the Raman spectra with both peak position and intensity and the infrared spectra with peak position. Additional information comprises the parameters of the calculation, to ensure reproducibility of the results.

The vibrational information makes the bulk of the database and constitutes the major computational effort. For each vibrational mode in the zone-center we determine the frequency, the symmetry assignment, the atomic displacement patterns, and the Raman tensors. The Raman spectra are represented in both single crystal and powder with different possible laser polarizations. For the infrared modes we give both the TO and the LO components.

The database is freely available on the web at http://www.wurm.info and is highly interactive. Jmol-powered applets incorporated in the website allow the quick visualization of the crystal structure and of the atomic displacement patters of all vibrational modes.

All the results are exclusively obtained from first-principles calculations performed using the local density approximation of density functional theory and density functional perturbation theory in the ABINIT implementation [http://www.abinit.org], based on planewaves and pseudopotentials.

After the brief presentation of the WURM project we focus on the potential to use the WURM database for identifying minerals based on their Raman signatures. We discuss at length the position of particular peaks associated with structural units, like the H_2O molecules or CO_3^{2-} SO_4^{2-}, PO_4^{3-}, etc anionic groups and the effect particular isotopic substitutions can have on the spectra. We analyze the behavior of the spectra along solid solutions, based on an alchemical pseudopotential technique.

Acknowledgements

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If interested, there are several ways of how anybody can get involved and provide support to our efforts: donate manpower, money, computing time, and expertise.

References

[1] Caracas, R. and Bobocioiu, E.: The WURM project - a freely available web-based repository of computed physical data for minerals, Amer. Mineral., 96, 437-443, 2011.