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The WURM project—a freely available web-based repository of computed physical data for minerals

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Abstract

The WURM project is a database of computed Raman and infrared spectra and other physical properties for minerals. The calculations are performed within the framework of the density-functional theory and the density-functional perturbation theory. The database is freely available for teaching and research purposes and is presented in a web-based format, hosted on the http://www.wurm.info web site. It provides the crystal structure, the parameters of the calculations, the dielectric properties, the Raman spectra with both peak positions and intensities and the infrared spectra with peak positions for minerals. It shows the atomic displacement patterns for all the zone-center vibrational modes and the associated Raman tensors. The web presentation is user friendly and highly oriented toward the end user, with a strong educational component in mind. A set of visualization tools ensures the observation of the crystal structure, the vibrational pattern, and the different spectra. Further developments include elastic and optical properties of minerals.

Keywords: Raman, infrared, density-functional theory, crystal structure, database, mineral physics, identification, dielectric