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A Large Database Of Raman Spectra Created With Optimized Computational Workflow

Abstract
Raman spectroscopy is a widely used material analysis technique based on the vibrational properties of materials. Raman spectra provide information about the vibrational modes, atomic structure, and chemical composition of materials but spectrographic analysis relies on comparison to known spectra. Hence, experimental databases of spectra have been collected but limited to well-known materials or the materials may contain significant amount of impurities of unknown identity, for instance.
The spectra can also be simulated using atomistic first-principles methods to complement experimental databases. However, current methods for the simulations of Raman spectra are computationally demanding. Thus, the existing databases of computational Raman spectra contain only a fairly small number of entries.
We present an optimized workflow to calculate the Raman spectra which can reduce the computational cost [1] and takes full advantage of the phonon properties found in existing material databases [2]. The workflow was benchmarked and validated by comparison to experiments and previous computational methods for select technologically relevant material systems.
Using the workflow, we performed high-throughput calculations for a large set of solid materials (5099) belonging to many different material classes and collected the results in a database that can be browsed online on the CRD website [3].

References

[1] M. Bagheri, H.-P. Komsa, Sci. Data 2023, 10, 80.
[2] A. Togo, Phonon database 2018, http://phonondb.mtl.kyoto-u.ac.jp
[3] M. Bagheri, H.-P. Komsa, Computational Raman Database 2023, https://ramandb.oulu.fi/

Figures

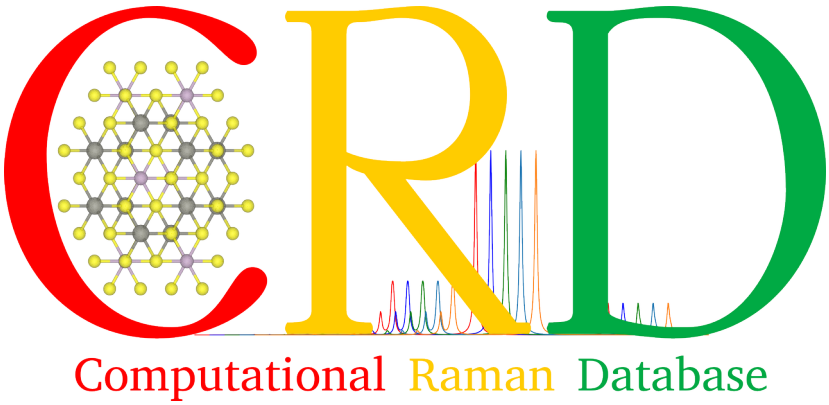

Figure 1: Computational Raman database logo