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Title: The VLab repository of thermodynamics and thermoelastic properties of minerals

Abstract

Thermodynamics and thermoelastic properties of minerals at planetary interior conditions are essential as input for geodynamics simulations and for interpretation of seismic tomography models. Precise experimental determination of these properties at such extreme conditions is very challenging. Therefore, ab initio calculations play an essential role in this context, but at the cost of great computational effort and memory use. Setting up a widely accessible and versatile mineral physics database can relax unnecessary repetition of such computationally intensive calculations. Access to such data facilitates transactional interaction across fields and can advance more quickly insights about deep Earth processes. Hosted by the Minnesota Supercomputing Institute, the Virtual Laboratory for Earth and Planetary Materials (VLab) was designed to develop and promote the theory of planetary materials using distributed, high-throughput quantum calculations. VLab hosts an interactive database of thermodynamics and thermoelastic properties of minerals computed by ab initio. Such properties can be obtained according to user's preference. The database is accompanied by interactive visualization tools, allowing users to repeat and build upon previously published results. Using VLab2015, we have evaluated thermoelastic properties, such as elastic coefficients (C_{ij}), Voigt, Reuss, and Voigt-Reuss-Hill aggregate averages for bulk (K) and shear modulus (G), shear wave velocity (V_s), longitudinal wave velocity (V_p), and bulk sound velocity (V_0) for several important minerals. Developed web services are general and can be used for crystals of any symmetry. Results can be tabulated, plotted, or downloaded from the VLab website according to user's preference.