

Polynomial fitting of stress-strain equations of state for crystalline materials

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We review in this contribution the techniques developed for the robust treatment of the static energy *\emph{versus}* volume theoretical curve [1]. These form part of our approach to the quasiharmonic approximation that let us predict thermodynamic elastic properties of crystalline solids to extreme pressures and temperatures. The case of MgO, Al, and diamond are discussed extensively.

References:

- [1] A. Otero-de-la-Roza and Víctor Luaña, *Comput. Phys. Commun.* **182** (2011) 1708--1720; 2232—2248.
[2] A. Otero-de-la-Roza and Víctor Luaña, *Phys. Rev. B* **84** (2011) 024109; 184103.