Influence of the exchange-correlation functional on the compressibility of solid mercury

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One of the key limitations of the density functional theory as an ab initio method is the independent particle approximation. This is compensated by the choice of a reasonable exchange-correlation functional that correctly describes the electronic subsystem and minimizes the calculation time simultaneously. Mercury is one of the most extraordinary chemical elements for simulations due to its complex electronic structure. Until now, there is no reliable model for obtaining the thermodynamic properties of mercury [1]. Obviously, for correct simulation, it is important to accurately take into account relativistic and correlation effects [2]. We obtained cold compression curves that are in good agreement with experimental data for the known solid-state phase of mercury using various exchange-correlation functionals, as well as some thermal properties. The possibility of calculations with the available functionals is treated.

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