Center for Molecular Modeling, Ghent University
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Technologiepark 903, Zwijnaarde

Prof. Dr. Piotr Spiewak

Warsaw University of Technology (WUT) / Faculty of Materials Science & Engineering

DFT prediction of the constant pressure heat capacity and thermal expansion tensor of materials

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DFT prediction of the constant pressure heat capacity and thermal expansion tensor of materials

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Thermodynamic properties are critical inputs for modelling a wide range of technologically relevant applications. The constant pressure heat capacity, $C_p(T)$, and the thermal expansion tensor, $\alpha_{ij}(T)$, play an important role in design of semiconductor devices as well as in thermophysical models of energy storage systems such as battery modules and proton exchange membrane fuel cells. In addition, $C_p(T)$ is an important component of constitutive models for forming of structural materials and phase diagram predictions. Density functional theory (DFT) can be used to compute these fundamental materials properties over broad temperature ranges using lattice dynamics based upon the supercell method. In the present study, we critically evaluate DFT predictions of $C_p(T)$ and $\alpha_{ij}(T)$ within the quasi-harmonic approximation for a range of crystalline materials. We selected specific metals, semiconductors, and insulators due to their significant technological relevance. In the case of the metallic systems (Al, Cu, W, La) $C_p(T)$ and $\alpha_{ij}(T)$ were computed with DFT using the LDA, PBE and PBEsol exchange-correlation functionals. The thermodynamic properties of semiconductors (Si, AlN, $CoSb_3$) and insulators (diamond, LiH) were evaluated additionally using the HSE range separated hybrid functional, which has been proven to yield properties of semiconductors and insulators in better agreement with experiment than standard local and semilocal exchange correlation functionals. For hexagonal crystal structures, the anisotropy of $\alpha_{ij}(T)$ was also investigated along with the temperature variation of the lattice constants. Theoretical predictions are compared with available experimental data.