Low Thermal Expansion of Layered Electrides Predicted by Density-Functional Theory

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Layered electrides are a unique class of materials with anionic electrons bound in interstitial regions between thin, positively charged atomic layers. While density-functional theory is the tool of choice for computational study of electrides, there has to date been no systematic comparison of density functionals or dispersion corrections for their accurate simulation. There has also been no research into the thermomechanical properties of layered electrides, with computational predictions considering only static lattices. In this work, we investigate the thermomechanical properties of five layered electrides using density-functional theory to evaluate the magnitude of thermal effects on their lattice constant and cell volumes. We also assess the accuracy of five popular dispersion corrections with both planewave and numerical atomic orbital calculations.

References

[1] Rumson, A. F., and Johnson, E. R., Low thermal expansion of layered electrides predicted by density-functional theory, *J. Chem. Phys.* **159**, 17 (2023).