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Computational methods in Materials Science studies

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Recent years have seen a great improvement in the field of Density Functional Theory (DFT) calculation of the structure and properties of crystalline materials. There are several reasons underlying the present successful application of DFT to materials science: Faster and faster computers, software improvements and theory advancement. Based on these three pillars, we the computing scientists are now fully able to understand the properties and performance of real materials. We are also able to explore the immense realm of the virtual materials in their quest for novel materials. Indeed, high-throughput techniques for the search of new crystal structures and the screening of band structure traits have become very popular in the field of computational materials science. Despite these, many challenges are still to be faced. Common to all computational materials scientists is the unquenchable thirst for higher speed and better accuracy in DFT calculations. This paper aims to present recent advances in the theory and computational methods in DFT calculation of materials as well as to highlight computational results on negative thermal expansion in cubic scandium triflouride in comparison to experimental and other theoretical studies.

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