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Cooperative Jahn-Teller effects in ScF3

Jahn-Teller effects arise in a crystal if distortions are considered on either the octahedral or tetrahedra complexes. This is a non-volatile approach in tailoring materials properties. ScF_3 is a material that has arouse special interests based on its Negative thermal expansion (NTE) behaviour. To this date, little is understood on the interplay between Jahn-Teller effects and NTE. The researchers herein, give a focus on how the Jahn-Teller interactions alter the chemistry of this crystal. We employed Density Functional theory as implemented in the {\sc Siesta} method coupled with mild distortions on the octahedra complex. The results herein go along way in exploring non-volatile approaches in engineering materials. Experimentalists can use this as a back bench in designing materials for novelty.
Key words: DFT, ScF3, NTE, Jahn-Teller distortions.

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