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Thermodynamic Stability and Vibrational Properties of Multi-Alkali Antimonides

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Modern advances in generating ultrabright electron beams have enabled significant experimental progress using synchrotron radiation. Current challenges include improving the quality of electron sources with novel photocathode materials such as alkali-based semiconductors. To fully harness their potential, a detailed characterization and prediction of their fundamental properties are essential. In this work, we employ density functional theory combined with machine learning techniques, integrated into the hiphive package, to probe the thermodynamic stability of various alkali antimonide crystals, emphasizing the role of the approximations taken for the exchange-correlation potential. Our results reveal that the SCAN functional offers an optimal trade-off between accuracy and computational cost in describing the vibrational properties of these materials. Furthermore, we find that systems with a higher concentration of Cs atoms exhibit enhanced anharmonicities, which are accurately predicted and characterized using our methodology.

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