

Abstract Submitted
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Lattice dynamics beyond the harmonic approximation: a compressive sensing approach FEI ZHOU, WESTON NIELSON, VIDVUDS OZOLINS, UCLA — First-principles modeling of materials in extreme conditions of increasing complexity has had profound impact on revealing and predicting the materials properties and explaining experimental results. Therefore methods and algorithms that can automatically scale to large systems with quantum mechanical accuracy are in dire need. Recently we have shown that a recently developed technique in the field of signal processing, compressed sensing (CS), provides a simple, general, and efficient way of constructing cluster expansion models for alloy systems. Here CS is applied to calculate force constants, including anharmonic effects up to high orders, in solids. CS performs well in extracting accurate lattice dynamics with highly competitive computational costs and reduced human efforts. Compressive sensing for lattice dynamics can be readily applied to much larger systems than ab initio methods can handle and with superior accuracy than classical force fields.

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