

Applications of Compressive Sensing Techniques for Materials Modeling



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Abstract:

The widely-accepted intuition that the important properties of solids are determined by a few key variables underpins many methods in physics. Though this reductionist paradigm is applicable in many physical problems, its utility can be limited because the intuition for identifying the key variables often does not exist or is difficult to develop. Machine learning algorithms (genetic programming, neural networks, Bayesian methods, etc.) attempt to help model building but often do so with increased computational burden and human time. A recently-developed technique in the field of signal processing, compressive sensing (CS), provides a simple, general, and efficient way of finding the key descriptive variables. CS is a new paradigm for model building. We demonstrate with the cluster expansion model and particularly the lattice dynamical model (CSLD) that CS is widely applicable, computationally efficient, systematically improvable and straight-forward to implement. This technical development is a big step towards systematic, automated calculations of thermodynamical and thermal transport properties for a wide variety of crystalline compounds, enabling computational design and discovery of new high-performance materials.

Biosketch:

Fei Zhou received his Ph.D. in physics from MIT in 2006. Dr. Zhou was a postdoc at MIT and an assistant research engineer at UCLA, before he joined the Lawrence Livermore National Lab as a staff physicist in 2013. His research is focused on computational materials science and materials physics for applications in electrochemical energy storage, nuclear fuel materials, thermoelectric materials, and rare earth materials for solid state lighting, radiation detection and permanent magnet.