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"Simple solutions to complex problems: high-throughput screening of novel ferroelectrics and thermoelectrics"

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First-principles, high-throughput screening of novel materials relies on our ability to calculate inexpensively and with predictive accuracy properties that are often very complex, and where established approaches require extensive human and computational effort even when dealing with a single system.
I will focus here on the phase stability of perovskite ferroelectrics and on the thermal conductivity of bulk and nanostructured thermoelectrics, showing in both cases how a combination of density-functional perturbation theory and few sprinkles of ingenuity can lead to inexpensive estimators of stability and performance.

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