Chris Marianetti, *A New Approach to the Interacting Phonon Problem*

Phonons and their interactions dictate many materials properties including phase stability, thermal transport, and mechanical behavior. Furthermore, there are various experimental phenomena related to phonon interactions, such as intrinsically localized modes, which lack a firm theoretical understanding but that could have technological relevance. Our research focuses on new techniques that can reliably treat the interacting phonon problem, accounting for both the classical and the quantum regime. We have developed the so-called Slave Mode Expansion, which delivers the anharmonic interactions from first-principles energetics, and we are now broadly applying this to prototypical crystals. In order to include quantum fluctuations, we are working on extending the dynamical mean-field theory (DMFT) to the interacting phonon problem. Success of our methodology could allow for applications spanning most material systems, ranging from transition metals in jet engines to actinides in nuclear fuels to hydrogen storage materials in fuel cells.