

Abstract Submitted
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Classical and quantum formalism of mode-based atomic-scale descriptions of lattice distortions K.H. AHN, JICHAN MOON, Department of Physics, Konkuk University, Seoul, South Korea — We present classical and quantum mechanical atomic scale theory of lattice distortions using atomic scale modes and their constraint equations. The formalism is demonstrated for a 1-dimensional chain and a 2-dimensional square lattice. We comment on the application of the mode-based atomic-scale approach for systems with strong anharmonicity and structural phase transitions.

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- [2] K. H. Ahn, T. Lookman, and A. R. Bishop, Nature 428, 401 (2004).

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