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Strain Engineering of the Electronic and Phonon properties of Lanthanum Monopnictides CHIA-MIN LIN, WEI-CHIH CHEN, CHENG-CHIEN CHEN, Department of Physics, University of Alabama at Birmingham — Rare-earth monopnictides have attracted significant attention due to their exotic electronic and topological properties with potential thermoelectric and spintronic applications. Here, we theoretically investigate strain effects on lanthanum monopnictides LaX ($X = \text{N, P, As, Sb, and Bi}$) by first-principles simulations using hybrid density functionals with spin-orbit coupling. In particular, the phonon properties, electronic bandstructures, and topological natures of these materials under compressive and tensile strains are computed. It is shown that strain engineering is an effective approach to manipulate the properties of LaX for improved performance and device applications.

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