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AELAS: Automatic ELAStic property derivations via high-throughput first-principles computation

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The elastic properties are fundamental and important for crystalline materials as they relate mechanical properties to thermodynamic ones, e.g., to the phonon dispersion and structural phase transformation. However, a complete set of experimentally determined elastic properties is only available for a small number of known materials. Therefore, an automatic scheme for the derivations of elastic properties that is adapted to high-throughput computation is much demanding. Here, we present the AELAS code, an automated program to calculate second-order elastic constants, moduli, anisotropy and phase stability criteria for both two-dimensional as well as three-dimensional crystal materials with any symmetry. The implementation of the code has been critically validated by a lot of evaluations and tests on a broad class of materials including two-dimensional and three-dimensional materials, providing its efficiency and capability for high-throughput screening of specific materials with targeted mechanical properties. As examples we demonstrate the AELAS capabilities for the three-dimensional structures, e.g., diamond and BN allotropes, and for the two-dimensional structures, e.g., the MXenes family.

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Refs

S. H. Zhang, R. F. Zhang, {\it AELAS: Automatic ELAStic property derivations via high-throughput first-principles computation}, Comput. Phys. Commun. {\bf 220}, 403–416 (2017).

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