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Objective structures. (English) [Zbl 1120.74312](#)
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Summary: An objective atomic structure is a collection of atoms represented by mass points or ions for which every atom sees precisely the same atomic environment, up to rotation (or, more generally, orthogonal transformations) and translation. An objective molecular structure is a collection of molecules in which corresponding atoms in each molecule see precisely the same environment up to orthogonal transformation and translation. Many of the most actively studied structures in science satisfy these conditions, including an arbitrary ordered periodic crystal lattice, the tails and also the capsids of certain viruses, carbon nanotubes, many of the common proteins and C_{60} . A single crystal rod that has been bent and twisted into helical form also satisfies the conditions in a certain sense. The quantum mechanical significance of objective structures is described and some general methods for generating such structures are developed. Using these methods, some unexpected objective structures are revealed. Methods for simplified atomic level calculations of the energy, equilibrium and dynamics of these structures are given.

MSC:

[74A25](#) Molecular, statistical, and kinetic theories in solid mechanics

Cited in **22** Documents

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Atomistic structures; biological material; numerical algorithms

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