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Novel approaches to ab-initio studies of materials at extreme conditions of high pressure and high temperature[1]

SERGEI SIMAK, Linkoping University

Theoretical description of thermodynamics, phase equilibria, and phase transitions in materials at high temperatures and pressures should include proper treatment of thermal motions of atoms. We show how this can be done in an accurate way within the modeling based on first-principles molecular dynamics. Our novel approach is illustrated by the examples ranging from elemental metals to superionic conductors.

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