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Ab initio modeling of electron subsystem of multiatomic crystals: software package. (English)

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Summary: A software package developed by the author is based on concepts of microscopic solid state theory and provides ab initio calculation of some fundamental aspects of multiatomic crystals. Results for *BaTiO3*, *PbMoO4*, and *GeTe* are in good agreement with available published experimental data.

MSC:

74N05 Crystals in solids
74-04 Software, source code, etc. for problems pertaining to mechanics of deformable solids
82D20 Statistical mechanics of solids

Keywords:

numerical modelling; band structure calculation; ferroelectric phase transition; pseudopotential method; total energy calculation

Software:

SCPPBAND