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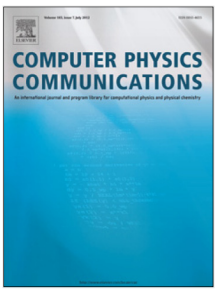

Large-scale *ab initio* simulations for periodic system

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Large-Scale *Ab Initio* Simulations for Periodic System

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In this manuscript, we present new capabilities and implementations on massively parallel computers of our *ab initio* orbital-free density functional theory software (ATLAS). In addition to the electronic ground-state capabilities, the extensive structure-related functionalities including geometrical structure relaxation and molecular dynamics simulation have been implemented in the new version of ATLAS. The effectiveness of these extensions is assessed through simulations of nanocrystalline and warm dense Al. The simulated results agree excellently with previous experimental and theoretical data, validating new capabilities. Furthermore, new version of ATLAS exploiting the massively parallel implementation with message passing interface shows high efficiency, as exemplified by its ability to simulate a system containing 4 million atoms only taking 1 hour with 2048 processors. The scalable parallel implementation of the ATLAS package with extensive capabilities holds considerable promise for simulation of large-scale systems with millions of atoms.

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