Abstract Submitted
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OWL: A scalable Monte Carlo simulation suite for finite-temperature study of materials[1] YING WAI LI, SIMUCK F. YUK, VALENTINO R. COOPER, MARKUS EISENBACH, KHORGOLKHUU ODBADRAKH, Oak Ridge National Laboratory — The OWL suite is a simulation package for performing large-scale Monte Carlo simulations. Its object-oriented, modular design enables it to interface with various external packages for energy evaluations. It is therefore applicable to study the finite-temperature properties for a wide range of systems: from simple classical spin models to materials where the energy is evaluated by ab initio methods. This scheme not only allows for the study of thermodynamic properties based on first-principles statistical mechanics, it also provides a means for massive, multi-level parallelism to fully exploit the capacity of modern heterogeneous computer architectures. We will demonstrate how improved strong and weak scaling is achieved by employing novel, parallel and scalable Monte Carlo algorithms, as well as the applications of OWL to a few selected frontier materials research problems.

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