Development of ab-initio configuration sampling toolkit (abICS) for combining first-principles calculations with extended ensemble methods

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In functional materials, varying types of configurational disorder are often employed to obtain favorable properties for a given application. The ability to simulate such disorder as a function of temperature should be immensely helpful for comparing with experiment. It would also enable prediction and design of properties in materials with realistic levels of disorder. To achieve this, a natural way may be to combine first-principles calculations with the Metropolis Monte Carlo algorithm. However, this is quite costly in terms of computational power, so many workers have opted to first derive lightweight models from first-principles calculations, then use that model for Monte Carlo sampling. The problem is that deriving lightweight *and* reliable models becomes increasingly difficult with increasing complexity of the system (various dopants, charged defects, interfaces, etc.).

In last year's ISSP joint-use project, SK proposed to bypass such fitting and instead rely on efficient parallel algorithms for thermodynamic sampling. Figure 1 shows our computational scheme. There are N_{rep} Metropolis samplers running in parallel at different temperatures. Each of the samplers spawns parallel DFT processes (we used VASP [1]) to perform local structural relaxation and energy calculation at every Metropolis step. The temperatures are swapped according to the replica exchange algorithm [2] to speed up the sampling. We successfully demonstrated that sufficient sampling can be performed on meaningfully large supercells by calculating the degree of disorder in $MgAl_2O_4$ [3].

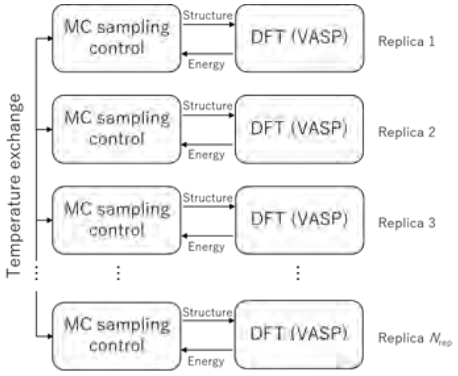

Figure 1 Our scheme for parallel configuration sampling. Reproduced from Ref. [3].

As this year's Software Advancement Project, we proposed to develop an easy-to-use interface for this computational scheme. The result has been released as ab-Initio Configuration Sampling toolkit, or *abICS* for short. It is written in Python 3 and is registered at PyPI (Python Package Index; pypi.org). It can thus be installed in most environments rather easily through the command "`pip install --user abics`". Now, abICS can sample using the replica exchange Monte Carlo algorithm, and we are planning to add support for other extended ensemble methods soon. The parameters for the sampling are controlled by an input file in TOML format, which is a minimal and easy-to-read configuration format that is being used in many software projects [4]. The parameters for the DFT calculations such as k-point sampling, basis set specification, convergence parameters, etc. are controlled by input formats of the specified solver. As the solver, abICS supports the use of DFT codes VASP, Quantum Espresso [5], and OpenMX [6] as of May 2020. It also has experimental support for aenet [7], which uses neural network potentials. Preprocessing scripts are provided for converting structure files to abICS input.

We believe that abICS will be immensely useful for making efficient use of next-generation supercomputers due to its multi-layered parallelism. We are also aiming to bring together information science, materials simulation, and statistical physics using abICS as a hub. Because of modular coding practices employed in our project, it should be relatively easy to implement interfaces for other solvers, or to implement new sampling schemes. Please have a look at our homepage [8] and do not refrain from contacting us if you are interested in using or extending this software.

References

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