

October 10, 2022

Dear Associate Editor Prof. Taylor Spark,

We are submitting our exciting contribution titled “***kMCpy: A Python Package to Simulate Transport Properties in Solids with Kinetic Monte Carlo***” to *Computational Materials Science*.

Understanding the kinetic processes in materials is crucial for technological applications, such as energy storage, catalysis, solid-oxide fuel cells, as well as crystal growths. Typically, these processes have been addressed using both molecular dynamics and kinetic Monte Carlo (kMC). However, the kMC approach appears less straightforward to implement because it needs: i) a comprehensive workflow to enumerate all possible transition events, ii) to construct a model to compute transition rates with high efficiency while bearing accuracy comparable to *ab initio simulation*, and iii) a robust kMC solver to propagate the simulation system as a function of time.

Here, we present a package named *kMCpy* to address the aforementioned requirements in addition to some unique features:

1. **Improvable lattice Hamiltonian:** *kMCpy* combined a rigorous formalism to compute transition rates based on a (local) cluster expansion theory, which is derived from first-principles calculations.
2. **Pythonic:** *kMCpy* is a modulus and highly customizable package fully developed using the versatile *python* language.
3. **Cross Platform:** *kMCpy* supports most mainstream platforms including Windows, macOS, and Linux, in both x86/64 and ARM architectures.
4. **Ease of Use:** All input and output data are supplied using human-readable JSON format, which is easily parsed and generated by computers. Furthermore, JSON is compatible across different platforms and hardware architecture.
5. **Performance:** The computationally-intensive routines of *kMCpy* are translated into optimized machine code at runtime using the *Numba* library.

We believe *kMCpy* and its implemented workflow provides a framework for the scientific community to predict the kinetic properties of any crystalline materials from first-principles calculations with high accuracy and performance. It is our belief that this work will be of significant interest to the readership of *Computational Materials Science*.

We confirm that this manuscript is not being simultaneously submitted to or under current consideration by any other journal.

Yours sincerely,
Pieremanuele Canepa on behalf of the authors