October 10, 2022

Dear Editor-in-Chief Professor Susan Sinnott,

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

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

Therefore, in this paper, we developed a package named *kMCpy* to cover these key points with following features:

1. **Pythonic**: *kMCpy* is a modulus and highly customizable package fully developed using *python*.
2. **Cross Platform**: *kMCpy* supports most mainstream platforms including Windows, macOS, and Linux, in both x86/64 and ARM architectures.
3. **Ease of Use**: All input and output data are supplied using human-readable JSON format, which is easily parsed and generated by computers.
4. **Performance**: The computationally-intensive routines of *kMCpy* are translated into optimized machine code at runtime using *Numba*.

We believe *kMCpy* and its implemented workflow will provide a framework to the scientific community to predict the kinetic properties of any crystalline solid materials from first principle with high accuracy and performance, and this work will be of great interest to the readership of *Computational Materials Science*. The following files are submitted on the website portal:

1. Manuscript
2. Cover letter
3. Source code of kMCpy

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