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Peer Review

Review of: "PyMatterSim: a Python Data Analysis Library for Computer Simulations of Materials Science, Physics, Chemistry, and Beyond"

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Here, I review the first preprint (version v1) of the manuscript titled *'PyMatterSim: A Python Data Analysis Library for Computer Simulations of Materials Science, Physics, Chemistry, and Beyond.'* In this manuscript, the authors introduce a Python tool for analyzing data from simulations of glassy materials. In my view, this tool has significant potential and could be highly relevant to the materials science community interested in glasses. I decided to provide my feedback separately on the tool and the written form of the manuscript.

Considering the tool:

Although I have not tested it, the GitHub repository for the tool and its accompanying documentation appear well-organized. The repository includes installation instructions and examples. A brief look at the code revealed extensive docstrings and the presence of tests implemented by the authors. Additionally, the file structure of the repository seems logical. Overall, the implementation leaves a positive impression, at least at first glance.

Considering the manuscript:

I recommend major revisions to the manuscript in its current form. I largely agree with the comments in the existing review by Marco Bertani[1] and would like to add a few additional points:

- I concur with the other reviewers that parts of the manuscript are overly wordy. Since the authors are presenting a tool for the analysis (postprocessing) of simulation data, it is unnecessary to describe MD simulation methods in such detail. Similarly, other sections reproduce textbook

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knowledge that could instead be cited. As a result, despite its length, the manuscript provides relatively little information about the software package being published.

- Additionally, the manuscript is lacking in citations: the first page of text includes only a single citation (in the first sentence, which conveys little substance). The introduction as a whole contains very few references, apart from a somewhat arbitrary selection of self-citations that are weakly connected to the context. For a paper with roughly 19 pages of text, citing only 42 references is surprisingly low.
- The authors also fail to present any results obtained using their tool, nor do they provide performance benchmarks, which would be a valuable addition to the publication. Furthermore, the manuscript does not compare their tool with others of similar purpose. Are there truly no comparable tools for analyzing such simulations? For instance, what about *matscipy*?"

Minor points:

- As mentioned in other reviews, Figure 1 appears to be cut off.
- In the introduction, the authors claim that there are only two classes of materials: crystals and glasses. While I understand that the tool is designed to analyze these two types of materials, for completeness, the authors should acknowledge the existence of other material classes.
- When discussing classical computer simulations, the authors state that simulation systems typically contain ~10^4 particles. However, with modern hardware, this number can now be orders of magnitude larger nowadays, particularly for standard MD simulations.
- The figure caption for Figure 2 lacks detail and could be more descriptive...
- Throughout the manuscript, equations are referenced by numbers, but the equations themselves are not numbered.

References

1. ^*Marco Bertani. (2025). Review of: "PyMatterSim: a Python Data Analysis Library for Computer Simulations of Materials Science, Physics, Chemistry, and Beyond". doi:10.32388/9bveho.*

Declarations

Potential competing interests: No potential competing interests to declare.