## Qeios

### Peer Review

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

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Having been involved in the development of analysis software, I was quite interested when I received an invitation to read this work. However, I was let down by a number of factors:

- The title is misleading: from what I was able to gather from the manuscript and from the GitHub repo, PyMatterSim is a collection of materials-science-specific analysis algorithms of MD trajectories focused on glass simulations coupled to some convenience converters for interchangeable use of different simulation sources. This seems to be useful in itself, but the title hints at a much broader use.
- The manuscript does not acknowledge important existing work. Python packages such as mdtraj or MDAnalysis should at the very least be mentioned (mdtraj is even an optional dependency of PyMatterSim, so the authors are clearly aware of its existence). More importantly, mdtraj or MDAnalysis could have actually been used as a basis on which to implement the analyses in this paper. This would save a lot of common boilerplate code dedicated to dealing with trajectory parsing and multi-format compatibility. Additionally, and also in this spirit, the manuscript makes little or no mention of API design decisions or extensibility. At the very least, some examples showcasing potential uses of the package should have been included.
- The objective of the manuscript quickly becomes unclear: it reads as a review of MD simulation and analysis methods. Many of the concepts that are described are not directly relevant to analysis

implementation in PyMatterSim. In addition, several of the concepts are presented in very general and not very accurate terms, meaning their description isn't useful neither as a review nor as an introduction to PyMatterSim.

• The use of AI-generated content could be acceptable if it enriched the narrative or the descriptions. Fig. 1, where the authors acknowledge AI use, does none of that (and that besides the obvious issues with the rendering itself). On the contrary, I'd argue Fig. 1 muddles the concepts the authors attempt to describe.

The rather careless use of AI in Fig. 1 also gives a strong suggestion that similar tools were used in the rest of the writing, which may explain some or all of my issues in the above points.

### Declarations

Potential competing interests: No potential competing interests to declare.