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Peer Review

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

Marco Bertani[1]

1. Università degli Studi di Modena e Reggio Emilia, Modena, Italy

The manuscript presents the PyMatterSim package developed to perform static and dynamical analysis of MD simulations.

It is always useful to develop new tools for data analysis, and this work can be helpful for the community. Anyway, some problems with the manuscript should be resolved, in my opinion.

- I think that there is a general lack of references in the manuscript. For example, when discussing interatomic potentials for glasses, the most used ones should be cited (PMMCS, SHIK, Edén, BMP, MLP...) and the same for rare events, where enhanced sampling methods are poorly referenced (see, for example, Lodesani et al).
- Figure 1 is not clear and is cut off at the border; consider changing it.
- In my opinion, several parts of the manuscript are too descriptive, and the authors tend to overdetail. As an example, the explanation of molecular dynamics is too long.
- The authors should explain what the “industrial standard” is that they cite.
- I think that a comparison to other programs in terms of the kind of analysis that can be done and computational cost should be reported, as well as the results on a simple well-known system like amorphous SiO2.

I think that overall, this work can be useful, and I hope the authors will continue their work to update the program.

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Declarations

Potential competing interests: No potential competing interests to declare.