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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The paper reports a novel Molecular Dynamics simulation engine in Python designed for non-crystalline materials where the analysis tools/theories (of primary importance in these kinds of systems) are well described.

I suggest some corrections to improve the quality of the paper and to make the software more easily usable by the community (and easier to be employed):

1. Why should one use pymattersim instead of Lammps or another package? What are the benefits? Or what can pymattersim do that others cannot?
2. A test case should be reported, a very well-known glass (oxides, chalcogenides, etc.) to show the capabilities (bond order, nematic order, etc.).
3. Are some force fields included in the package? If yes, please give the list. If not, add a way to include the force field that the user needs.
4. How much faster is it with respect to other packages (not only for MD but also in the analysis)? Probably for these glass-like systems, Lammps is the reference.
5. Regarding the analysis tools, I can suggest reading the paper about analysis tools for short- and medium-range order in disordered systems (*ACS Omega* 2022, 7, 27, 23255−23264).
6. Figure 1: OK, that has been made with AI. It seems also pretty cool, but it is cut at the borders (two-body and many-body). Two-body is referred to distances, three-body to angles, and four-bodies to dihedrals. Probably it is better to insert these labels.

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Declarations

Potential competing interests: No potential competing interests to declare.