

Peer Review

Review of: "Machine Learning of Slow Collective Variables and Enhanced Sampling via Spatial Techniques"

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The manuscript reviews machine learning-based techniques for identifying slow collective variables (CVs), focusing on methods exploiting the spatial characteristics of the data. The manuscript is very well written, and the literature review is extensive. Consequently, I only have one point that I suggest the authors address:

1. One way to overcome the chicken-and-egg problem is to design/discover transferable CVs, at least for some particular chemical sub-space or application. The authors should address the transferability aspect of CVs, include recent work in this area (e.g., <https://doi.org/10.26434/chemrxiv-2024-1xhm0>), and discuss current issues and future perspectives.

Declarations

Potential competing interests: No potential competing interests to declare.