

Peer Review

Review of: "Comment on “Exploring potential energy surfaces to reach saddle points above convex regions” [J. Chem. Phys. 160, 232501 (2024)] by M.Gunde et al."

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The authors commented on a recently reported study on convex regions of potential energy surface (PES). In contrast to the activation-relaxation technique nouveau (ARTn), in this work the authors apply the theory of Newton trajectories (NTs) to the 2D PES. This work concerns a mathematical detour which discusses the use of the ARTn for the PES with various convex regions. I do not recommend this work for publication until the authors largely revise and polish this manuscript.

First, I cannot get the point of this paper. By abstract, I think the authors may comment on convex regions of PES by NTs by comparing with ARTn. However, in the first few line of the Introduction section, the authors seem to forget what they said about NTs in abstract. Then, the authors throw out Equations (1) and (2) for mechanochemistry. Finally, the authors again forget them in Section II. Therefore, I do not understand authors' goal in this comment. The present manuscript seems to be a note of reading reference. The authors may want to be further polish it.

Second, the authors reported that NTs are able to calculate for the PES of Frenkel-Kontorova chains with up to 500 atoms and for medium molecules with up to 150 atoms. I cannot get what means by authors' statement. This is not surprising because power of NTs has been well-known by chemists. As far as I know, NTs in conjunction with a statistical ensemble have capability to simulate systems with

$10^4 \sim 10^5$ atoms.

Third, the authors seem to concern on simulations of mechanochemistry and thus Equations (1) and (2) become important in this manuscript. However, the PES means electronic-energy function of nuclear coordinates. It seems to be too phenomenological to study physics/chemistry insights by adding a force term on PES. The authors may give much more improvement or perspective on this issue. On the other hand, the present benchmark is a 2D PES which is too simple as an example. Since NTs are performed, I think a much more high-dimensional PES or a realistic PES should be used to show the power of the authors' calculations.

Declarations

Potential competing interests: No potential competing interests to declare.