

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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I am not an expert in the relevant field, so I just comment on the paper's content from a general perspective.

The author applied the Newton trajectory approach to the 2D PES problem for finding saddle points. The problem was used as a toy problem studied by M. Gunde et al. using ARTn. In general, I do not doubt that the NT approach shows advantages in this particular system. However, to demonstrate the utility of this method, the authors should consider more complicated, high-dimensional problems. Since the EOM in NT uses the Hessian, which is very expensive to calculate for high-dimensional problems, as already mentioned by the authors, I suggest the authors also comment on the computational cost and provide an overall justification of the NT approach based on the test results for more complicated examples.

Declarations

Potential competing interests: No potential competing interests to declare.