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Efficient minimum mode finding in transition states calculations
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— Transition states are fundamental to understanding the reaction dynamics qualitatively in chemical physics. To date various methods of first principle location of the transition states have been developed. In the absence of the knowledge of the final structure, the minimum-mode following method climbs up to a transition state without calculating the Hessian matrix. One weakness of this kind of approaches is that the number of rotations to determine the minimum mode is usually unpredictable. In this work, we propose a locally optimal search direction finding algorithm which is an extension of the traditional conjugate gradient method without additional calculations of the forces. We also show that the translation of forces improves the numerical stability. Experiments for the Baker test system show that the proposed algorithm is much faster than the original dimer conjugate gradient method.

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