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Potential Energy Surfaces, NewtonTrajectories and Optimal Oriented External Electric Fields

Abstract: The talk begins with a discussion of Newton trajectories (NT). An NT is a curve where the gradient of the PES points in the same direction at every point. NTs connect stationary points of the PES, so they can be used to find saddle points. Application: NTs describethe curves of the change of stationary points under a mechanochemical or electric force. A special application is the study of the smallest amplitude electric field that renders a barrierles chemical process with the smallest possible strength. For this we search for an optimal bond breaking point. An example PES is explained.

References:

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