Car-Parrinello and path integral molecular dynamics study of the hydrogen bond in the chloroacetic acid dimer system.

Autorzy

Piotr Durlak

Carole A. Morrison

D. S. Middlemiss

Zdzisław Latajka

Rok wydania

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Streszczenie

We have studied the double proton transferDPTreaction in the cyclic dimer of chloroacetic acidusing both classical and path integral Car-Parrinello molecular dynamics. We also attempt toquantify the errors in the potential energy surface that arise from the use of a pure density functional.In the classical dynamics a clear reaction mechanism can be identified, where asynchronized DPTarises due to coupling between the O–H stretching oscillator and several low energy intermolecularvibrational modes. This mechanism is considerably altered when quantum tunneling is permitted inthe simulation. The introduction of path integrals leads to considerable changes in the thermallyaveraged molecular geometry, leading to shorter and more centered hydrogen bond linkages

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