

Car-Parrinello simulation of an O-H stretching envelope and potential of mean force of an intramolecular hydrogen bonded system: application to a Mannich base in solid state and in vacuum.

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Streszczenie

Car-Parrinello molecular dynamics (CPMD) study was performed for an anharmonic system—an intramolecularly hydrogen bonded Mannich-base-type compound, 4,5-dimethyl-2(N,N-dimethylaminemethyl)phenol, to investigate the vibrational spectrum associated with the O-H stretching. Calculations were carried out for the solid state and for an isolated molecule. The classical CPMD simulation was performed and then the proton potential snapshots were extracted from the trajectory. The vibrational Schrödinger equation for the snapshots was solved numerically, and the (O-H) envelope was calculated as a superposition of the $0 \rightarrow 1$ transitions. The potential of mean force for the proton stretching mode was calculated from the proton vibrational eigenfunctions and eigenvalues incorporating statistical sampling, nuclear quantum effects, and effects of the environment. Perspectives for application of the presented methodology in the computational support of biocatalysis are given in the study.

Adres publiczny

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