Abstract

Two investigations of different characters are made in this work. The first concerns the vibrational energy transfer in ice Ih and the second is a theoretical investigation of compounds related to skin allergy. Density Functional Theory (DFT) has been the main correlation method used for the quantum chemical calculations performed throughout these studies. This thesis includes a short introduction to DFT, and also provides a base for the choice of Molecular Dynamics method, i.e. Car-Parrinello Molecular Dynamics (CPMD).

In our study, we used a cluster of 15 water molecules to model ice Ih, and simulated the excitation of the vibrational modes in the central water molecule using CPMD. The CPMD results suggest that the relaxation of the vibrational mode occurs within 100 femtoseconds. It also indicates that the excitation energy is transferred both intramolecularly and intermolecularly on approximately the same timescale. These results are compared with an earlier developed wavepacket approach on the same topic. And both approaches are in agreement with previously reported experimental results on an ultra-fast vibrational energy transfer in water. The background of vibrational energy transfer in ice together with the considerations for the theoretical model is also discussed in this thesis.

A different field of chemistry concerns oxidation of chemical fragrances and surfactants. The second part of this thesis joins computational calculations with previous and current experimental research. The studies focus on the activation of common non-allergenic compounds into skin sensitizers due to air-oxidation when these compounds are handled and stored. To identify substances that can cause contact allergy, experiments on animals are needed. The incorporation of computational chemistry aims to reduce the number of experiments on animals. In this thesis, the oxidation of common components of chemical fragrances and surfactants and their oxidation products have been investigated. Different oxidation mechanisms have been examined, and the oxidation products found in the experiments are discussed and confirmed in view of the calculated results. Hence, the computational approach is promising for predicting if a compound has an inherent propensity to become a skin sensitizer.

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