Theoretical study of infrared spectra of iodide molecules on NaCl surfaces

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ABSTRACT

Iodine, when released into the environment, contributes to the oxidizing capacity ofthe atmosphere through the catalytic destruction of ozone [1, 2]. Iodine-131 can be released during a severe nuclear accident and can be carcinogenic for humans [3]. In theliterature, there are missing pieces of knowledge about interactions between iodinated compounds and aerosols. In this context, this work consists in investigating the adsorption on sea salt aerosols of gaseous methyl iodide (CH_3I), diiodomethane (CH_2I_2), and water. We have used two different methods: a periodic approach using Quantum ESPRESSO [4, 5] and a cluster QM/QM' approach using the ONIOM method [6] from Gaussian 16 [7]. We have computed the adsorption energies and the shift in vibrational frequencies, due to adsorption. We have shown that the vibrational frequency shiftsare small, mainly because there is no strong coupling between the adsorbates and the NaCl(001) surface, as illustrated by the low values of the adsorption energies.

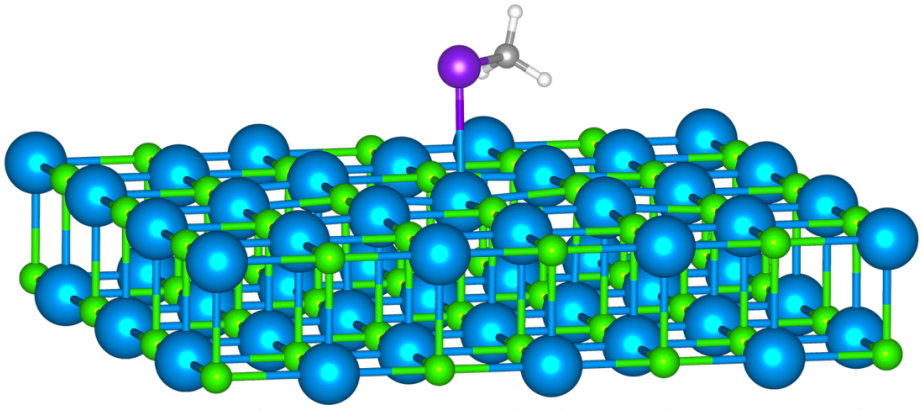

Figure 1: Optimized DFT geometry of CH_3I on a NaCl(001) surface from a QM/QM' ONIOM (DFT/PM7) calculation

References

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