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Modelling of the interaction of halogenated molecules with the ice surface

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The interaction between ice and halogenated species has received much attention in the past few years in the context of atmospheric chemistry and ozone depletion. Much theoretical and experimental work has been carried out in order to understand the HX (X=Cl, Br···) behaviour (adsorption or ionization) at the ice interface. Up to now, very few studies have been dedicated to photolytic processes occuring at the interface. The work we present here concerns the dynamics and the photodissociation of halogenated molecules (HCl, Cl2, CH3Cl···) adsorbed at the ice surface by means of classical and quantum dynamical calculations.

Please list some keywords

modelling, halogens, dynamics, photodissociation, adsorption

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