



# Interaction of Ozone and Water on Potassium Iodide Aerosols

Fayçal ALLOUTI, Sidi SOUVI, Alexis MARKOVITS, Florent LOUIS

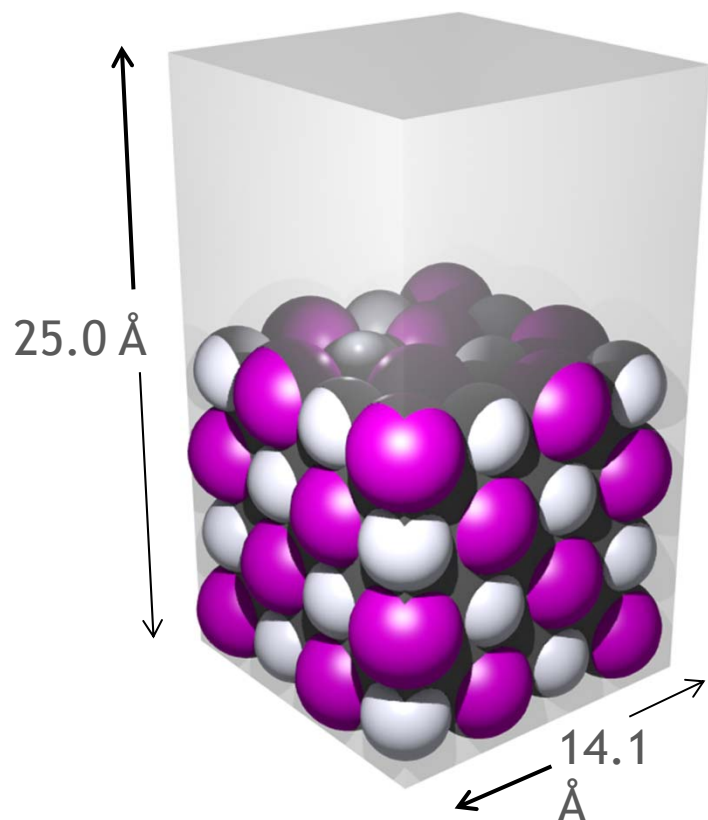


# Introduction

Experimental studies of ozone on a dry (100) KI show the formation of a passivation layer of  $\text{KIO}_3$ . This reaction initiates at step edges of the surface first and then spreads across the terraces [1,2]. Surface adsorbed water molecules induce a completely different reaction pathway that leads to the formation of gaseous iodide compounds [3].

To understand how humidity changes the reactivity of ozone towards KI surface, the interactions involved in these processes need to be investigated. This is what we are planning to do with computational chemistry.

# Computational Details



Periodic DFT calculations:

- VASP5.4 [4]
- Functional: PBE [5] with Grimme D2 correction
- Cutoff energy: 520 eV

- Cell dimensions:  $p(2\sqrt{2} \times 2\sqrt{2})R45^\circ$   
 $a = b = 14.1 \text{ \AA}$

- 2 frozen layers

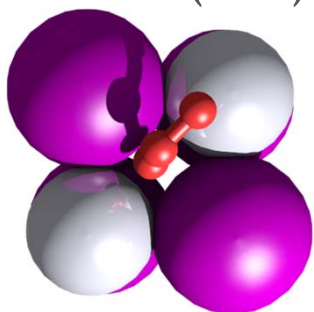
DFT calculations on molecules:

- Gaussian09 [6]
- Functional: PBE [5] with Grimme D2 correction
- Basis set: aug-cc-pVTZ

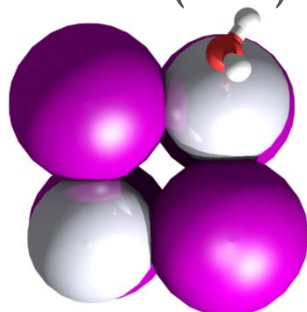
# Results

Single adsorption: (top views)

Ozone on (100) KI    Water on (100) KI



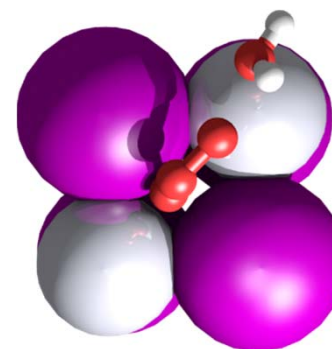
$$E_{\text{abs}} = -42.2 \text{ kJ/mol}$$



$$E_{\text{abs}} = -37.0 \text{ kJ/mol}$$

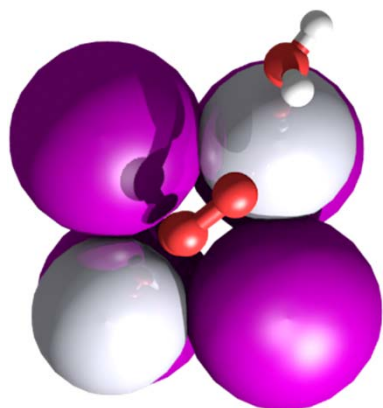


Coadsorption  
starting geometry:

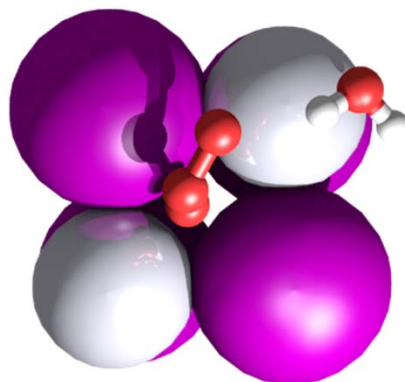


Coadsorption sites and energies: (top views)

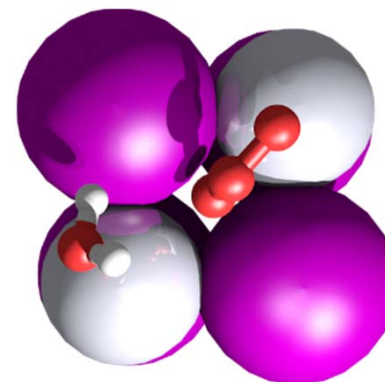
Site 1



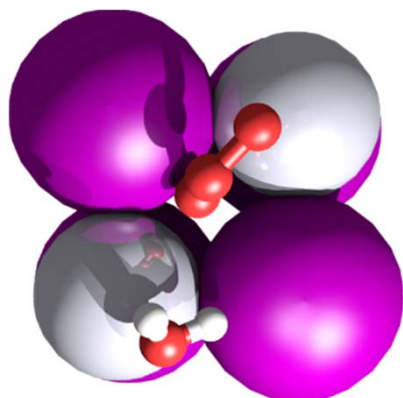
Site 2



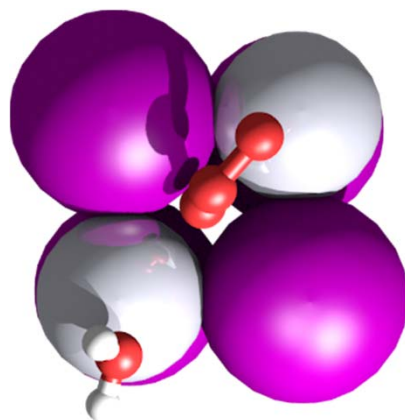
Site 3



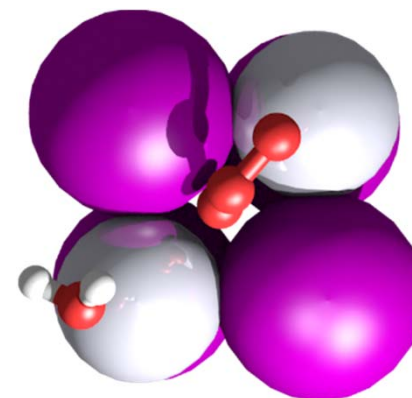
Site 4



Site 5

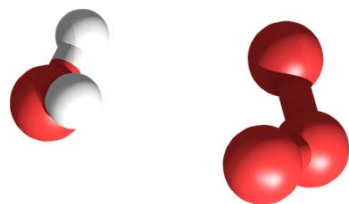


Site 6



kJ/mol	$E_{\text{ads}}(\text{H}_2\text{O}+\text{O}_3)$	$E_{\text{inter}}$	$E_{\text{ads}}$ of ozone on wet site
Site 1	-91.9	-12.7	-54.9
Site 2	-99.6	-20.4	-62.6
Site 3	-103.4	-24.1	-66.4
Site 4	-104.4	-25.2	-67.4
Site 5	-107.8	-28.6	-70.8
Site 6	-107.7	-28.5	-70.7

Ozone - water in gas-phase:



$$E_{\text{inter}} = -16.9 \text{ kJ/mol}$$

Ozone on a water-free (100) KI surface:

$$E_{\text{abs}} = -42.2 \text{ kJ/mol}$$

# Conclusions and Outlooks

Water plays a role at the first step of ozone interaction with the KI (100) surface. The adsorption is made easier on sites where a single water molecule is present. The interaction between ozone and water is increased by the KI surface.

## Outlooks

- Ozone interaction with higher water coverages,
- Further reaction steps on dry and hydrated surfaces,
- Adsorptions on step edges,
- Other alkali iodide particles that can be found in nuclear power plants such as NaI.