DIRECTION DES SCIENCES DE LA MATIERE,
INSTITUT RAYONNEMENT MATIÈRE DE SACLAY

SERVICE DE PHYSIQUE ET DE CHIMIE DES SURFACES ET DES INTERFACES

SEMINAIRE *

Thursday 12 novembre 2011 à 14h00

Bâtiment 466, salle 111 - CEA Saclay, 91191, Gif sur Yvette

Water adsorption on $BaTiO_3$ (001).

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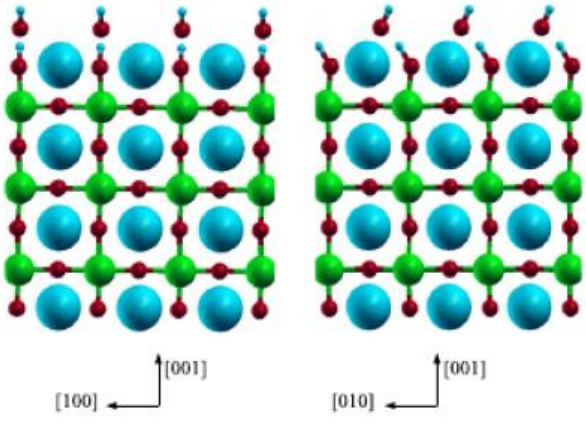
The adsorption and dissociation of water on $BaTiO_3$ (001) surfaces has been studied by density-functional calculations. It is found that such surfaces are strongly reactive with respect to water so that, in ambient conditions, they are probably fully hydroxylated. A state of molecular adsorption is found, distinct from simple physisorption, as already observed on some other perovskite surfaces such as $SrZrO_3$ and $SrTiO_3$. It is shown how the direction of the in-plane polarization and the adsorption might influence each other, leading to some surface imprint effect due to water. The results of related experiments are discussed, as well as the implications of such results on the screening mechanisms at ferroelectric surfaces.



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