Title : Theoretical study of the physical and optical properties of some metal oxide oxide surfaces for greenhouse gas sensing applications

First Name : Nathalie	**Name** : VAST	**Laboratory** : LSI

Email : nathalie.vast at polytechnique.edu

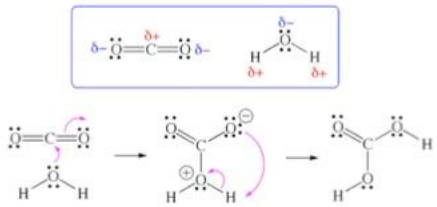
Webpage :

Research Area : Condensed Matter Physics, Materials Science

Methods: Optical response of materials will be in investigated in numerical simulations with methods based on the time-dependent density functional theory on which the host team has developed an expertise [1-3], as implemented in the QUANTUM ESPRESSO package [4]. Part of the project may consist in theoretical and numerical implementations.

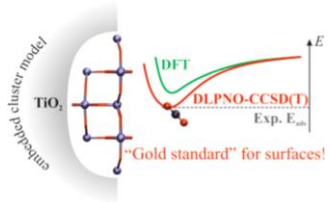
PhD track subject :

The research of processes to measure, capture, and dissociate greenhouse gases is often based on the gas photo-dissociation by metal oxide surfaces (MOSs) [5,6]. Surface defects, and in particular oxygen vacancies and charged trapped therein, play an important role in the (photo)reactivity of MOSs. However, the way optical properties are modified by such defects is not completely understood, nor is the additional effect of the presence of the gas. In the project, a special focus will be set on the determination of the optically properties of a MOS, for instance TiO_2 [7-10], eventually deposited on gold, and its interaction with a GHG like CO_2.



Schema of the chemistry of CO_2 dissociation in water

(From Shapley, http://butane.chem.uiuc.edu/pshapley/genchem1/l23/web-l23.pdf)



Potential of a triatomic molecule on a surface of TiO_2

(From. Ref. [11])

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