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Study of the adsorption of simple molecules on metal oxides by ab initio calculations: Application to the detection of gas

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The team "micro sensors" at the IM2NP mainly focuses on the development of gas sensors, whose principle is based on measurement of conductance variation in presence of gas. The material used as sensitive element is a semi-conductor metal oxide (WO_3 , Cu_2O or CuO) and target gas is a simple molecule such as ozone, NO_x or CO_x . The objective of ab initio calculations is to better understand the interactions between gas and oxide surface at atomic scale in order to propose possible improvements to the selectivity of these sensors. All systems have been simulated using the SIESTA code based on DFT. We present here some of results obtained on WO_3 surface and Cu_2O surface for ozone adsorption/dissociation. In the case of WO_3 , results for NO_x and CO_x molecules are exposed too.

Biography

Caroline Lambert-Mauriat is a Researcher at Aix-Marseille University, France. She is a Lecturer in Industrial Computing at the Institute of Technology of Aix-Marseille University. She has completed her PhD from the University of Aix-Marseille in Materials Sciences. Her main research interest includes "The study of oxide surfaces and their interactions with simple molecules by ab initio calculations".

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