Conception par calculs ab initio de matériaux optimisés pour l'énergie et l'environnement

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Nowadays the degree of sophistication of atomistic simulations based on density functional theory (DFT) is very high and "numerical experiments" can be realized [1-4]. These simulations can help to understand at a molecular level the interactions between molecules and materials. Combining different atomistic simulation techniques such as *ab initio* molecular dynamics with other theoretical methods and machine learning, one can accurately predict adsorption enthalpies of molecules in nanoporous materials. This allows a fast screening of a large number of formulations to design efficient and materials with optimized properties for various applications. We will give some applications of these modeling tools for the selective capture of radioactive iodine in case of nuclear severe accident [2] and for the production of biofuels from biomass waste [3,4]. Surface or catalytic reaction mechanisms can be also computed to identify the key steps in a specific process [5]. In close connection with experiments, the use of *ab initio* modeling open the path to an integrated approach for the development of optimized nanomaterials and processes in the fields of catalysis and environment.

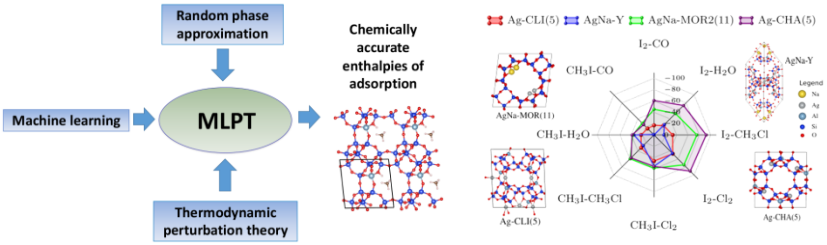

Figure: Machine Learning Perturbation Theory / Radar plot for screening adsorbents

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[5] J. Quílez-Bermejo, A. Daouli, M. Badawi, V. Fierro et al. Advanced Functional Materials 33 (2023) 2300405.