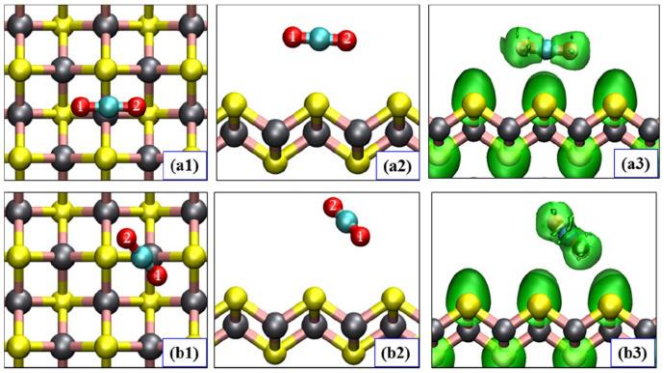
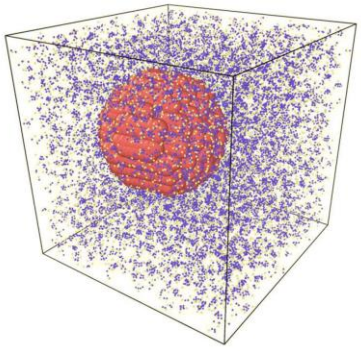
Multi-scale (DFT and MD) Computational Modeling:

Multi-scale computational modeling combines existing and emerging methods from various scientific disciplines to bridge the broad range of time and length scales that are inherent in a number of essential phenomena and processes in materials science and engineering. A correct understanding of electronic-structure-scale (DFT) and molecular-scale (MD) is necessary to describe the physics and chemistry that govern the properties and processes of materials under realistic temperature and pressure conditions.



DFT



MD

What the Student Will Do in The Project:

The student will study profoundly the density functional theory (DFT) and Molecular Dynamics (MD) methodology. The student will perform multi-scale computational modeling to understand how molecules (e.g., CO_2, H_2, CO) interact with solid surfaces (i.e., TiO_2). In this context, DFT and MD simulations can contribute to this understanding by addressing the following questions:

1-Where will the molecule adsorb?
2-How many molecules will stick to the surface?
3-What is the adsorption energy?
4-What are the mechanism of adsorption?
5- ...

Required from the Student:

Background in materials physics (solid state physics), and interest in materials science will be an advantage. We need a student interested in computational modeling, and working independently in a larger group of scientists. An interest in computational methodology based on the DFT and Molecular MD is required. Experience with C++ or Python and previous knowledge with the basics of DFT and MD will provide a good starting point for further learning.

Other Aspects:

This topic is closely related with the other research projects in MPT. This project will be in close collaboration with Prof. Jrg Neugebauer director of the Computational Materials Design department of the Max Plank Institute for Iron research in Germany, and Prof. Anthony Paxton from Theory and Simulation of Condensed Matter research group in King's college London will be actively involved in this project.

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