Master Physics & Computational Physics
1st year project (2020-2021)

Title: Molecular dynamics simulation of the adsorption of oxygen on a copper surface

Key words: gas-surface reactivity, classical trajectory method, atomic adsorption, energy dissipation

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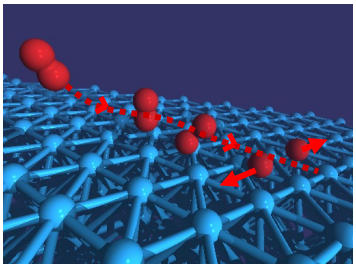
Subject :

Gas-surface heterogeneous processes play an important role in many reactive processes. Indeed, reactions involving heterogeneous catalysis represent 90% of industrial chemical processes (ammonia synthesis, producing hydrocarbon…). These processes are also an integral part of the chemistry occurring in the atmosphere (clouds formation, soot aging, etc.) or in the interstellar medium through the reactivity on grains of carbonaceous dust.



Another example where gas-surface reactivity is important is the atmospheric re-entry of space vehicle. During atmospheric re-entry of a planet, the space vehicle is subjected to a significant rise in temperature induced in part by adsorption and recombination phenomena of gaseous species on the heat shield. These catalytic processes would represent 30% of the total heat flux received by the vehicle wall. In this context, understanding the elementary gas-surface mechanisms (adsorption, absorption, recombination, etc.) is essential.

In this project, we propose to study **the adsorption of oxygen on a copper (100) surface**, oxygen being one of the elements mainly affecting the atmospheric re-entry on Earth. The primary objective of the project will be to build a molecular dynamics code suitable for the study of an atom/surface process (based on pre-existing codes). For the O/Cu (100) system, a good quality potential energy surface is available in the laboratory. It will therefore then be possible to characterize the mechanisms of oxygen adsorption on the metal surface as well as the dissipation of its incident energy towards the atoms of the surface.

***Numerical tools*:** fortran/python/bash scripts
Equipment: PC, computer cluster (mésocentre UFC)