Séminaire de Chimie Théorique

Salle conférences 3eme Est, Bat. A12
Mardi 1 Octobre à 11:00

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Adsorption dynamics of simple molecules on surfaces from first principles

Since the mid 90s, it has become possible to carry out realistic classical and molecular dynamics simulations of adsorption of simple molecules on surfaces from first principles calculations.
In this seminar the basic method used at present in the field of gas-surface dynamics will be described. As an illustration, some new results for dissociative adsorption of molecular hydrogen on Pd/Ru and Pd/Cu bimetallic surface alloys and methane on Pt(111) and Ni(111) will be presented.

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