





Martedì 18 febbraio 2025 alle ore 14:30 presso l'aula F del DiSC

la Prof. Marialore Sulpizi

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terrà il seminario dal titolo:

The electrified platinum/water interface

from ab initio and machine learning simulations

Atomistic mass and charge distribution at electrified interfaces play a key role in electrochemical phenomena of huge technological relevance for energy production and conversion. However, in spite of its importance, the structure of the double layer at the nanoscale is still to a large extent unknown, even for Pt-water, the most fundamental electrochemical interface.

In this seminar I will present our recent results from ab initio simulations of the Pt-water interface under applied potential, revealing charge spillover, oscillation, and changes in water adsorption, which in turn influence the interface capacitance.

I will also discuss the role of hydrogen adsorption at varying of the applied potential and how the coverage modulates the interfacial water behavior.

Finally, I will present the equilibrium structure of the electric double layer at a defective platinum/electrolyte interface also including the acid dissociation equilibrium. Here machine learning potentials have permitted us to push time boundaries and to address larger and more complex models at the nanosecond time scale. Challenges, limitations and perspectives will be also discussed.

La presenza della S. V. sarà molto gradita

Il Direttore del Dipartimento Stefano Mammi

Alberta Ferrarini