nanoX invited scientist

Llinersy URANGA PINA

Position Full Professor

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Host lab at NanoX LCAR Team Theory

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Dates of stay February 14th, 2022 - April 13th, 2022

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Brief Biodata

Prof. Llinersy Uranga Pina completed her Ph.D at the University Paul Sabatier and the University of Havana in 2012. She developed teaching, research and supervision activities mainly at Latin American and European universities and research institutions (e.g., University of Havana, National University of Quilmes, Free University of Berlin, Abdus Salam International Centre for Theoretical Physics). Since 2017 she holds a full professorship in theoretical physics at the University of Havana, where she leads a research group on molecular physics. She has been awarded the Young Scientist Award (Caribbean Academy of Sciences), the Annual Prize of the Cuban Academy of Sciences, Distinction of the Cuban Minister of High Education, among other recognitions.

Research project during the visit at nanoX

Trajectory-based approach to quantum dynamics at the nanoscale

The project aims to investigate archetypal dynamical processes of atoms and molecules in the vicinity of nanostructured surfaces (e.g., quantum scattering and diffusion). Methodologically, we will use and further improve our previously developed quantum trajectory representation. Dynamics at surfaces will be treated within a rigorous quantum approach, which keeps the appealing intuitiveness of classical mechanics by representing the time evolution of a quantum probability distribution as a swarm of interacting trajectories. The project aims to overcome practical difficulties which are ubiquitous in modern computational tools for the study of quantum dynamics (e.g., the use of large grids or basis sets, the challenge to account simultaneously for bound and unbound wavepacket dynamics). It will improve the accuracy, numerical stability and scalability of quantum dynamical simulations, thus enabling to address quantum phenomena in nanoscale systems which lie at present out of the scope of the nowadays standard simulation techniques. As first applications, we will focus on the theoretical description of the translation inelasticity upon collision of H with pristine and H-covered tungsten surfaces, and the hydrogen adsorption in nanoporous materials. Implications for hydrogen storage and isotope separation via quantum sieving will be considered.

If relevant, add a figure

Legend