NANOSCIENCE COLLOQUIUM

Weakly Bound Materials: Competing Energy Scales, Quantum Effects and Machine Learning

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A B S T R A C T : Weakly bound systems, comprising molecular materials, vdW heterostructures and interfaces between different material components, give rise to a rich variety of nuclear motion and tuneable nuclear structures that are tightly connected to diverse electronic properties in these systems.

In this contribution, I will discuss how we push the limits of density-functional theory and different ab initio techniques that capture nuclear motion to unravel the properties of realistic interfaces.

I will give an overview of simulation methods that are applicable for large system sizes and that can capture the quantum nature of nuclei in anharmonic potential energy landscapes,as well as what the inclusion of non-adiabatic effects in these simulations entails.

I will discuss how machine-learning techniques can speed up the computation of nuclear and electronic properties, allowing larger and more accurate simulations that can reach thermodynamic limits of first-principles accuracy.

I will finish by showing a couple of applications where the quantum nature of the nuclei becomes indispensable to assess the structural and electronic properties of 2D materials and interfaces.

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