Hybrid Inorganic/Organic Systems for Opto-Electronics

Collaborative Research Centre 951

Colloquium Announcement

of the Collaborative Research Centre 951
"Hybrid Inorganic/Organic Systems for Opto-Electronics"

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Stacking van der Waals atomic layers: quest for new quantum materials

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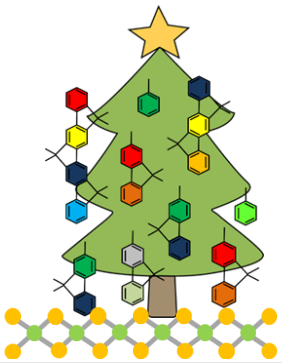
Simulating nuclear motion and their impact in hybrid organic-inorganic systems



Time: Thursday, 17.12.2020, 15:15

Place: The colloquium takes place online (ZOOM)

Meeting-ID: 687 6163 8786
Password: 951951

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Stacking van der Waals atomic layers: quest for new quantum materials

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Modern electronics heavily rely on the technology to confine electrons in the interface layers of semiconductors. In recent years, scientists discovered that various atomically thin van der Waals (vdW) layered materials can be isolated. In these atomically thin materials, quantum physics allows electrons to move only in an effective 2-dimensional (2D) space. By stacking these 2D quantum materials, one can also create atomic-scale heterostructures with a wide variety of electronic and optical properties. We demonstrate the enhanced electronic and optoelectronic performances in the vdW heterostructures, suggesting that these a few atom thick interfaces may provide a fundamental platform to realize novel physical phenomena. In this talk, we will discuss several research efforts to realize unusual quasiparticle pairing mesoscopic devices based on stacked vdW interfaces between 2-dimensional materials.

Simulating nuclear motion and their impact in hybrid organic-inorganic systems

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Weakly bonded interfaces, commonly encountered in hybrid organic-inorganic architectures, give rise to a rich variety of nuclear motion and tunable nuclear structure that is 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. We show that the level alignment at interfaces containing soft organic materials like pentacene strongly depend on the structure and strain of the interface [1]. In addition, anharmonic nuclear motion is shown to be tightly related to the properties of singlet fission in the organic crystal [2]. In contrast, in weakly bonded interfaces where ground state electronic charge transfer (CT) takes place, the balance between molecule-molecule and molecule-surface interaction [3] can be decisive for the atomic and electronic properties. Additional CT, promoted by electronic excitation, from the inorganic to the organic component in similar interfaces are weakly impacted by vibronic couplings [4]. However, in the case of vdW heterostructures based on transition metal dichalcogenides, we show that vibronic coupling plays a key role in the temperature dependence of the ground-state CT across the components [5].

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[3] H. Wang, S. V. Levchenko, T. Schultz, N. Koch, M. Scheffler, and M. Rossi,
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