

Why nanostructures are different?

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KEYWORDS: *Nanostructures, Moire bilayers, correlated electron-ion dynamics, anharmonicity.*

In my talk I will give a general introduction to vibrational properties, and their coupling to electron liquid, in nanostructures. In the first part I wish to provide a brief and accessible explanation on what happens when a characteristic size of a device reaches an order of nanometers. I shall introduce concepts such as energy level quantization, surface-to-volume ratio, anharmonicity and non-adiabaticity to discuss their implications and range of applicability. To be specific I shall focus on one- and two-dimensional systems where collective phenomena definitely determine the physics of the material. These are the systems that are at present at the forefront of materials science such as nanotubes, nanorods, stepped surfaces, but also topological states on crystal dislocations. One particular example that I will explore in more detail are Moire bi-layers.

The reason why Moire bi-layers are special is because at a finite twist angle, in a single sample one obtains a set of atoms with varying degrees of anharmonicity and non-adiabaticity. Indeed, several exotic orderings have been detected in this platform within the last decade of intense research, which has lead to numerous publications in the highest level journals. Thus, in the second part of my talk I will show how to incorporate such extraordinary lattice dynamics within a full microscopic quantum mechanical description: the method of effective correlated electron-ion dynamics (ECEID). I will present the ECEID equation (together with a sketch of their derivation) and compare the results with simpler methods for instance Ehrenfest dynamics.

In the last part of my talk I will show how these microscopic results can be employed into a field theoretical description of nanostructures at the mesoscopic scale. It is at this scale that the collective phenomena play a crucial role and ought to be captured. In this way measurable quantities can be obtained. Overall, the aim of this talk is to show that a description of materials that include the quantum mechanical effects is entirely possible already with a current state of knowledge. Importantly, up to large extend it does not require a heavy numerical effort, but it is a description that uses analytical methods.

ACKNOWLEDGEMENT:

I acknowledge collaboration with my PhD student Shaswati Mandal on a part of the ECEID computations, and interesting discussions on numerical implementations with prof Wacław Kuś and prof. Tadeusz Burczynski. We acknowledge financial support of NCN under OPUS grant no.2021/43/B/ST8/03207