Carl von Ossietzky
Universität
Oldenburg
Institut für PHYSIK

PHYSICAL COLLOQUIUM

INVITATION

Monday, 12.07.2021, 4.15 p.m.,
video conference: https://meeting.uol.de/b/anj-2vc-j6s-fwe

speaks

Prof. Dr. Caterina Cocchi,

Institut für Physik, Theoretische Festkörperphysik, Universität Oldenburg

about

"Electronic structure theory for future: New opportunities for old challenges"

The development of non-polluting materials for efficient harvesting, conversion, and storage of renewable energies is one of the challenges of this century. As the driving effects of these functionalities are quantum mechanical in nature, the role of electronic structure theory is crucial to disentangle the underlying processes and to interpret them. First-principles methods have been successfully employed for material characterization for a few decades. However, problems related to light-matter interaction and, more generally, to the description of excited-state properties, have suffered until very recently from limited computing power and from the lack of efficient algorithms. State-of-the-art computing architectures finally enable the quantitative description of electronic, optical, vibrational excitations and their combined dynamics in real materials. Furthermore, recent developments of automatized computational infrastructures and data repositories have introduced the new paradigm of computationally-aided research which bridges the incoming era of artificial intelligence.

In this lecture, I will discuss how these opportunities can help us concretely to develop new materials and, in this way, to address some of the challenges of our times. In particular, I will highlight the current activities of my group in the development and characterization of advanced systems and nanostructures for renewable energy generation, conversion, and storage. With the aid of selected examples, I will show how first-principles electronic structure theory can complement experiments in various fields, ranging from chemistry to accelerator physics, to understand and predict structures, properties, and functionalities of the materials of tomorrow.

All interested persons are cordially invited.

Sgd. Prof. Dr. Caterina Cocchi