

Fritz-Haber-Institut der Max-Planck-Gesellschaft

Physikalische Chemie — Direktor: Prof. Dr. Martin Wolf



MAX-PLANCK-GESellschaft

Department Seminar:

Monday, May 28, 2018, at 11:00 a.m.;

— all are invited to meet at around 10:40 for a chat and coffee —

Prof. Dr. Caterina Cocchi Theory of excitations in low-dimensional systems,
Department of Physics & IRIS Adlershof,
Humboldt-Universität zu Berlin.

Light-matter interaction at the nanoscale: What can we learn from first-principles calculations?

PC Seminar Room G2.06, Building G, Faradayweg 4

R. Ernstorfer

Abstract:

Understanding the fundamental physical mechanisms of light-matter interaction at the nanoscale is a crucial task for controlling and predicting the response of materials to electromagnetic radiation. First-principles methods based on density-functional theory and many-body perturbation theory are particularly suited to complement experiments in order to interpret and predict the laboratory observations. As they do not rely on external empirical parameters, these approaches are able to describe physical phenomena in their full complexity without any a priori assumptions. From a theoretical viewpoint, the main challenges are related to correctly capture correlation effects and to provide a comprehensive description of the response of the systems also beyond the linear regime. In this seminar, I will introduce these methods and demonstrate their predictive power in the appropriate physical contexts. With the examples of technologically relevant systems, including organic semiconductors and van der Waals materials, I will show how first-principles methods offer physical insight into light-matter interaction processes complementary to experiments..