Dresden University of Technology

Faculty of Physics

# PHYSICS COLLOQUIUM

*Speaker:*

**Prof. Simone Sanna**
Institut für Theoretische Physik,
Justus-Liebig-Universität Gießen

*Topic:*

**Modeling the linear and nonlinear optical response of condensed matter from first principles: From monolayers to ferroelectric structures**

*Time and place:*

Tuesday, December 9, 2025, **2:50 pm** – hybrid event
**The colloquium will be held in REC/C213.**
Online participation possible:
Zoom-Meeting: Meeting-ID: 631 3817 8900 / passcode: PC-WiSe25
https://tu-dresden.zoom-x.de/j/63138178900?pwd=TlmGawPz1dtDA6VzO2N1XdqqI7bE6b.1

*Host:*

Prof. Lukas Eng

*Abstract:*

Modeling the linear and nonlinear optical response of complex systems from first principles is one of the most challenging tasks in theoretical materials science. How is it possible to predict the outcome of the light-matter interaction for a system of $10^{23}$ particles, only from the basic laws of quantum mechanics and electrodynamics? In this colloquium, we will take a journey into classic and innovative approaches in atomistic materials modelling, discussing capability and actual limits of computational physics. In particular, a novel approach based on the calculation of the dynamical polarization is introduced, which is applied to cutting-edge research topics at the TU Dresden. The presented methods allow both to understand the outcome of experimental investigations as well as to identify the relationships between composition, morphology and the macroscopic material properties. In turn, this paves the way for computer-supported material design, inspiring the realization of real structures with tailored properties.

*Bio:*

Simone Sanna is professor for theoretical physics at the Justus Liebig University in Giessen, where he leads the research group theoretical solid-state spectroscopy. With his team, he performs quantum mechanical simulations to predict the physical properties of complex material systems on the basis of their microscopic structure. Besides developing first-principles computational approaches to model spectroscopic signatures, AI based models are applied for the interpretation of imaging spectroscopy results. Ferroelectric oxides, optically nonlinear molecular clusters and on surface molecular synthesis are in the focus of the research.