HYP*MOL

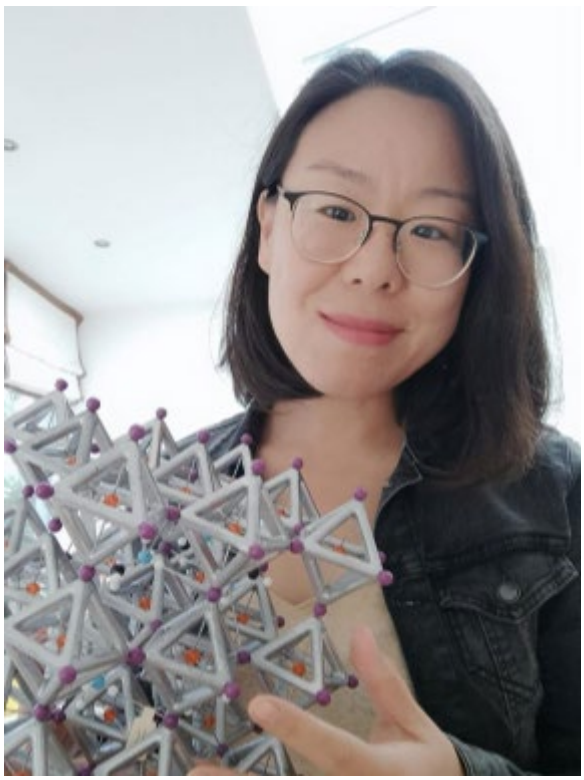
HYPERPOLARIZATION
IN MOLECULAR SYSTEMS

TRR-386

DFG Deutsche Forschungsgemeinschaft

Joint Colloquium of the TRR-386 and the Institute of Physics

Hörsaalgebäude, TU Chemnitz, Reichenhainer Straße 90
10 July 2025, 15:30 h, N013



Prof. Dr. Shuxia Tao

Eindhoven University of Technology

Materials theory of halide perovskites

Halide perovskites are a versatile class of materials with tunable photonic, electronic, and spin-related properties, making them promising for applications from solar energy to quantum technologies. Their soft, ionically conductive lattice and chemical flexibility enable tailored functionalities and seamless device integration. Our group applies first-principles simulations and machine learning to uncover the structure–property relationships that influence performance and stability.

A key focus is the chemistry and physics of defects, which play a central role in long-term stability. We model defect formation and migration pathways, and propose strategies such as compositional tuning and surface passivation. In parallel, we explore chirality in hybrid perovskites, examining how chiral ligands induce spin-selective effects like chiral induced spin selectivity (CISS) and enhance chiroptical responses, paving the way for spintronic and chiral optoelectronic devices.

15.00 h pm there will be coffee and cookies in front of the lecture hall. For more information about this event, please ask Prof. Dr. G. Salvan, salvan@physik.tu-chemnitz.de or 0371-531-38319