Max-Planck-Institut für
Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

IMPRS UFAST Call for PhD applications 2023/2024

GB1-Vibrational properties of nanostructures: from ab-initio to semiempirical approaches.

Title of PhD Project	**Vibrational properties of nanostructures: from ab-initio to semiempirical approaches.**
Type	Theory
Supervisor(s)	Prof. Gabriel Bester, Dr. Torben Steenbock
Affiliation(s):	Hamburg University
Number of positions:	1
Abstract:	Understanding the vibrational properties of materials becomes crucial as temperature deviates from absolute zero. Vibrations play a pivotal role in how materials interact and behave thermally, impacting various aspects of their functionality. Well-established theories on vibrations exist, primarily from the physics community for bulk materials and from quantum chemists for small molecules. In this project, we target an intermediate scale, situated between individual molecules and bulk materials—the realm of nanostructures. Nanostructures possess unique vibrational characteristics that differ from bulk materials and individual molecules. Our objective is to bridge this theoretical gap by utilizing established methodologies and innovating new approaches. Drawing upon our recent advancements, this project will amalgamate knowledge from both physics and quantum chemistry domains. We will apply our methodology to colloidal nanostructures and 2D twisted (Moire) systems. This deeper comprehension will not only contribute to fundamental science but also pave the way for technological advancements and applications in various fields, such as nanotechnology and quantum information science.
Contact person for scientific questions about the project:	Prof. Gabriel Bester: Gabriel.bester@uni-hamburg.de