Max-Planck-Institut für
Struktur und Dynamik der Materie
Max Planck Institute for the Structure and Dynamics of Matter

IMPRS ULTRAFAST IMAGING & STRUCTURAL DYNAMICS

IMPRS UFAST Call for PhD applications 2021/2022

Novel wavefunction-based simulation methodology for a unified treatment of quantum structure and dynamics in extended systems
A. Rubio-4

Title of PhD Project	**Novel wavefunction-based simulation methodology for a unified treatment of quantum structure and dynamics in extended systems.**
Type	Theory
Supervisor(s)	Asst. Prof. Aaron Kelly, Dr. Guillermo Albareda, Prof. Angel Rubio
Affiliation(s):	Max Planck Institute for the Structure and Dynamics of Matter Dalhousie University University of Barcelona University of the Basque Country
Number of positions:	1
Abstract:	The goal of this project is to develop and apply novel wavefunction based simulation techniques to address nontrivial quantum mechanical phenomena in correlated electron-ion systems. Our group has recently developed a conditional wavefunction theory that allows for a fully quantum mechanical description of the structure and dynamics of molecular systems. The developmental side of this project will focus on the extension of conditional wavefunction theory to treat periodic systems, and these developments will be incorporated within the Octopus software package. This framework will then be applied to simulate response, relaxation, and transport phenomena in molecular and extended systems such as 3D solids, and 2D heterostructures. Examples of interest include simulating nonlinear phenomena such as phonon-assisted optical activity, photoinduced charge transfer, and the behavior of light-induced topological states.
Contact person for scientific questions about the project:	Aaron Kelly: aaron.kelly@mpsd.mpg.de Guillermo Albareda:guillealpi@gmail.com Angel Rubio: angel.rubio@mpsd.mpg.de

CFEL SCIENCE · DESY. · Universität Hamburg DER FORSCHUNG | DER LEHRE | DER BILDUNG · European XFEL · MAX-PLANCK-GESELLSCHAFT