DYNASTY

DYNAmics and STructural analYsis of 2D materials

DYNASTY WORKSHOP

Wednesday 05/04/2023, 15:00

STEP-C Saitakis Room

Introduction to Pybinding and Quantum-Kite

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Abstract:
In the first part of the workshop, I will give an overview of the Pybinding [1] and Quantum-Kite [2] tutorials, starting with an introduction into tight-binding and spectral methods, and continuing with a description of the functionalities and strengths of each code and scenarios on where the codes can be of great use in the description of opto-electronic properties of 2D materials. In the second part, I will present hands-on tutorials in the form of Jupyter notebooks containing Pybinding scripts that will introduce most of the functionalities of the software. Finally, I will present examples from the Quantum-Kite package [3], which uses Pybinding as an interface and allows for efficient simulations of large-scale disordered systems.

References:

[1] Pybinding website: https://docs.pybinding.site/en/stable/

[2] Quantum-Kite website: https://quantum-kite.com/

[3] KITE: high-performance accurate modelling of electronic structure and response functions of large molecules, disordered crystals and heterostructures, SM João, M Anđelković, L Covaci, TG Rappoport, JMVP Lopes, A Ferreira, Royal Society Open Science 7, 191809 (2020)

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