DYNASTY

DYNAmics and STructural analYsis of 2D materials

DYNASTY WORKSHOP

Thursday 06/04/2023, 12:00
FORTH Payatakes Room

Modelling phonons in nanomaterials and calculation of the Huang-Rhys factor and the photoluminescence spectra

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Abstract:
The vibrational properties of nanomaterials play fundamentally important roles in determining their stability and various functionalities, from the rippling of otherwise flat two-dimensional (2D) monolayers to the extreme thermal transport behaviors observed in one-dimensional (1D) and 2D carbon-based systems. Here we discuss modeling efforts to understand how phonons in lower dimensional materials differ from those in bulk, and how these behaviors manifest in their unusual properties. This workshop will discuss important phonon calculation details from first principles methods related to nanomaterials with hands-on examples on hBN/MoS_2. In the latter portion of the workshop, we will use the calculated phonon properties for the estimation of the Huang-Rhys factor and photoluminescence spectra of the defect state. This method can be used to identify novel materials for room-temperature quantum photonics with applications in single-photon emitters.

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