DYNASTY

DYNAmics and STructural analYsis of 2D materials

DYNASTY SEMINAR

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FORTH Seminar Room 1

Strain gradient in low dimensional materials and its effect on optoelectronic and flexoelectric properties

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Abstract:
Flexoelectricty is the coupling of polarization and strain gradients, which can be detected by bending a material. Flexoelectricity can be found in a wide range of materials, including soft matter, liquid crystals, and crystalline materials, although it is only noticeable at short-length scales, where strong strain gradients emerge. In this talk, I'll discuss recent developments in the computation of optoelectronic and flexoelectric properties under strain gradient using first-principles approaches. Furthermore, flexoelectric properties of rippled monolayer InSe and MoS_2, using the density functional theory and phenomenological Landau approach will be discussed. In these monolayers, the flexoelectric effect outperforms the piezoelectric effect in both in-plane and out-of-plane directions. A realistic strain gradient of roughly ~ 1 nm^{-1} can induce an order of magnitude higher flexoelectric response than the piezoelectric one. These findings will be discussed in the context of recent experimental measurements.

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