

Fracture of 2D Materials – In situ TEM Experiments and MS Parameterized Force Fields

Horacio Espinosa

Northwestern University

ABSTRACT

2D materials are being employed in the development of next-generation electronics, optical, and sensor technologies, as well as in energy production and storage techniques, e.g., supercapacitors, solar cells, and battery electrodes. Such applications involve frequent mechanical deformations such as stretching and bending, so the materials' lifespan (integrity and reliability) is a critical feature. In this context, the abrupt and brittle failure of 2D materials requires particular attention. In this presentation, I will discuss strategies for the in-situ electron microscopy fracture testing of 2D materials and advances in the parameterization of interatomic potentials (force fields) for accurately describing crack tips' atomic lattice reconstructions and bond dissociations. Experimentally, I will discuss e-beam-assisted crack propagation with measurement of crack tip deformation fields, based on atomic images, and computation of toughness. The parameterization of force fields is based on a multi-objective genetic algorithm and machine-learning-inspired protocols, with training and screening data sets involving both equilibrium and far-from-equilibrium pathways such as phase transitions, vacancy formation energies, and bond dissociation energy landscapes. Using monolayer MoSe₂ as a testbed, I will illustrate the effectiveness of the combined experimental-computational approach in measuring and predicting the toughness of the material, demonstrating in the process the advantages of ML-inspired force field parameterization in developing computational approaches with predictive capabilities.