

# UMENO LAB.

## [Multiscale Simulation of Strength and Property of Materials]

Center for Research on Innovative Simulation Software

Nanostructured Materials Strength and Science

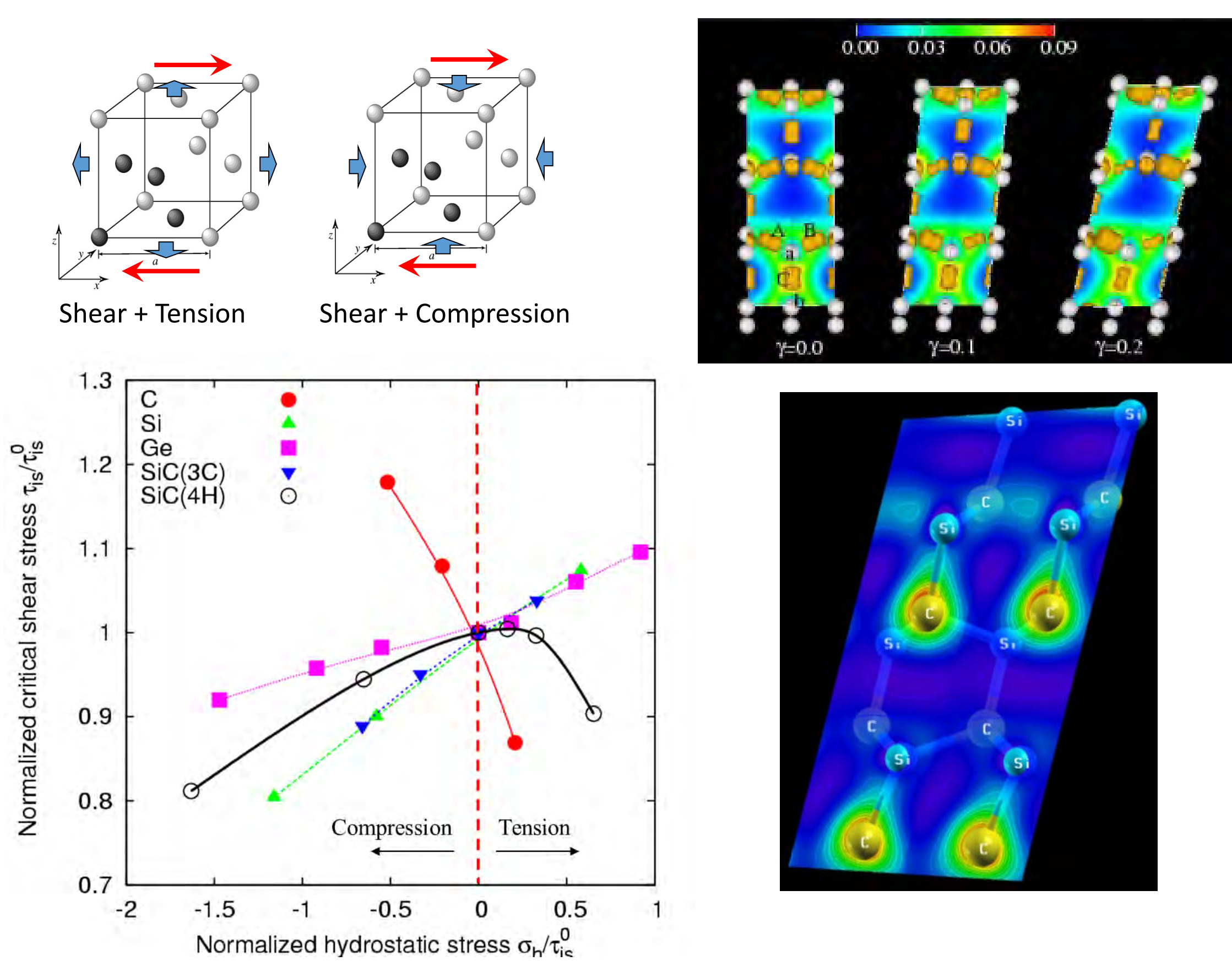
Dept. of Mechanical Engineering

<http://www.cmsm.iis.u-tokyo.ac.jp>

### Theoretical Prediction of Strength and Physics of Nanomaterials and Multiscale Simulation

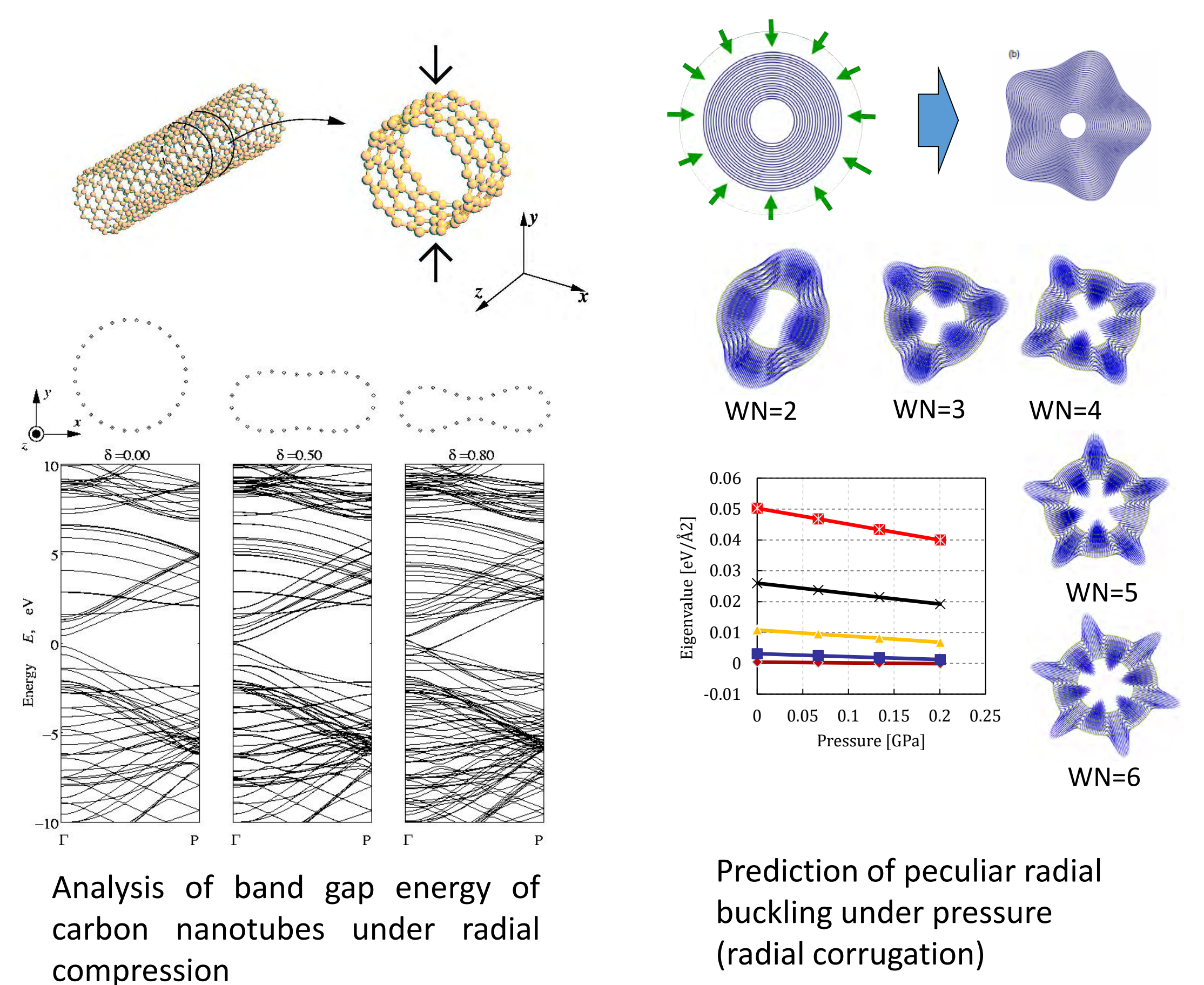
We aim to reveal the mechanical and physical properties of nanomaterials by ab initio density functional theory calculations and molecular dynamics simulations. We also work on multiscale simulation based on knowledge of nano-microscale phenomena.

#### Effect of normal stress on ideal shear strength

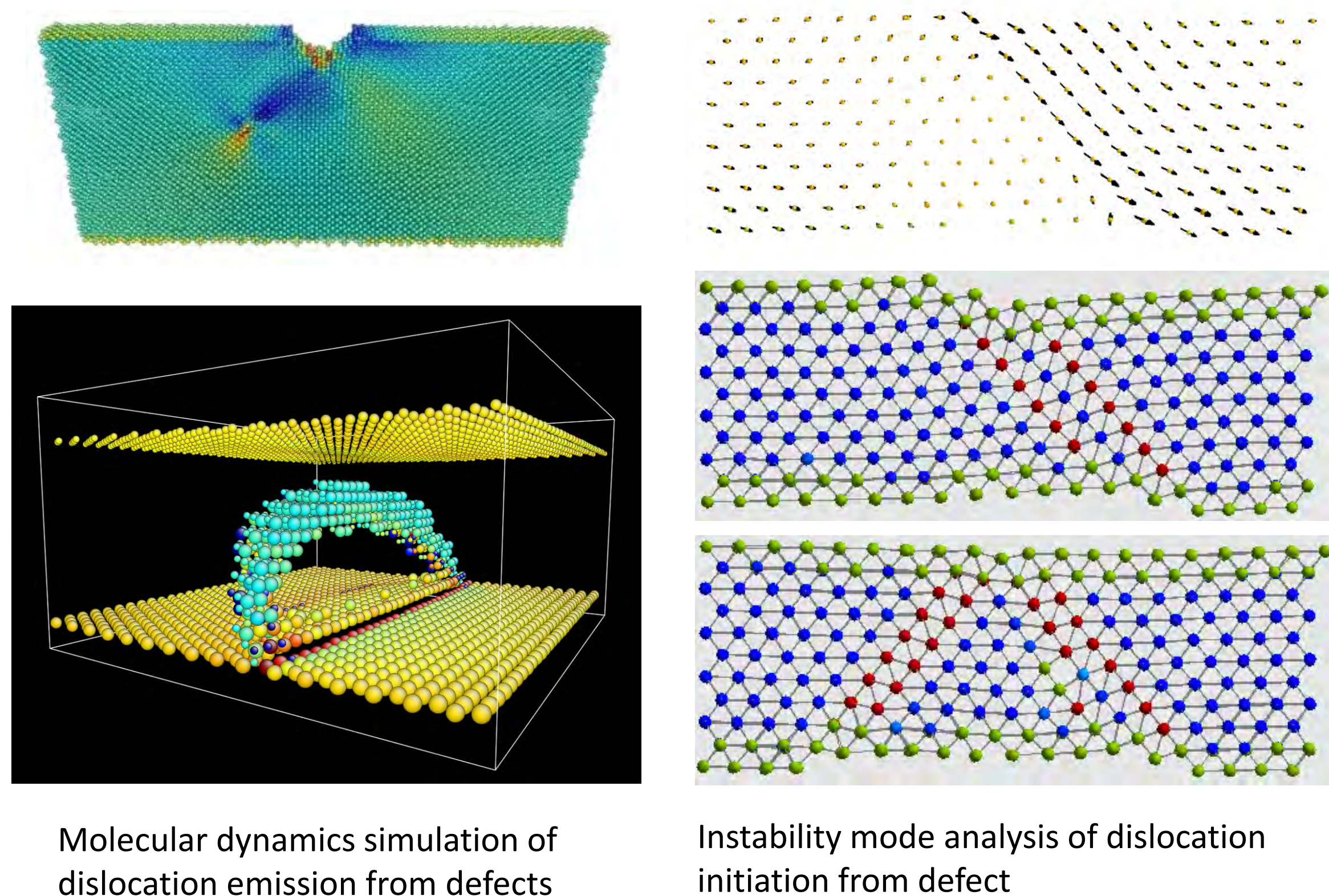


Ideal shear stress (ISS) under compression/tension, which is important to interpret experiments (e.g. nano-indentation tests), has been calculated. Response of ISS qualitatively differs. Note that compression always increases ISS in metals.

#### Compression of carbon nanotubes



#### Atomic structure instability analysis



#### Multiscale simulation of polymer materials

