

## UMENO LAB.

Challenges to Nano-Micro Mechanophysics  
and Multiscale Simulation

Department of Fundamental Engineering

Nano-Micro Mechanophysics

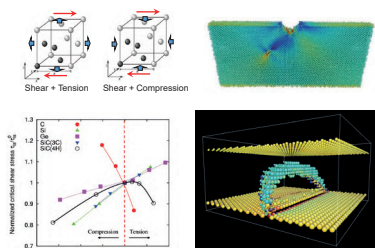
Department of Mechanical Engineering, Graduate School of Engineering

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

## Unveiling Nano-Micro Mechanophysics for hierarchical Multiscale Simulation

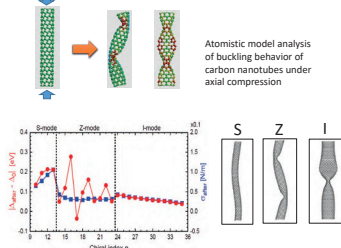
We aim to reveal the mechanical and physical properties of nanomaterials by ab initio density functional theory calculations and molecular dynamics simulations. We also work on multiscale simulation based on knowledge of nano-microscale phenomena.

### Atomistic simulation of crystal deformation and fracture



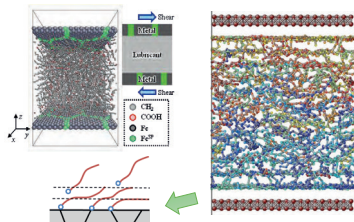
Ideal shear stress (ISS) under compression/tension in covalent crystals

### Designing nanodevice utilizing buckling deformation



Nanotube diameter vs. buckling mode, buckling-induced band gap change, and post-buckling stress

### Molecular simulation of boundary lubrication



### Multiscale simulation of polymer materials

