



# Laboratoire de Mécanique des Solides

CNRS UMR 7649, X, Mines  
École Polytechnique - 91128 Palaiseau Cedex  
Tél. 01.69.33.57.03 (secrétariat) - Fax : 01.69.33.57.08



## Séminaire du LMS

Jeudi 22 Mars 2018

14<sup>h</sup>00

Salle Jean Mandel

**Pr. Kyung-Suk KIM**

Brown University

### **Critical curvature localization in graphene used for molecular informatics: The graphene moleculography**

Imaging of molecules and/or nano-particles at the atomic level, correlating it to their functionalities, has been elusive. Here, we report “graphene moleculography,” a novel scientific method that provides the ability to investigate physical and/or chemical phenomena using only small number of molecules at the atomic scale. The moleculography is composed of (i) a “graphene molecular zipper” (GMZ) for alignment and manipulation of molecules on a graphene surface, (ii) AFM-based “graphene atomic lattice interferometry” (G-ALI) to resolve the molecular structure and its interaction state, and (iii) computational algorithms for the molecular informatics of G-ALI. Similar to the historical scientific-advancement example of X-ray/crystallography pair, the G-ALI/moleculography pair has potential to advance molecular science and technology with unprecedented resolution and versatility.

In this talk, analysis of critical curvature localization in graphene caused by quantum flexoelectricity is emphasized in the discussion to explain our discovery of graphene crinkles used in GMZ design. The GMZ utilizes invariant-mode bifurcation of multi-layer graphene crinkle, which creates flexoelectric charge concentration within sub-nanometer bandwidth along the crinkle ridges and valleys. Controlling the charge potential depth, the charge localization acts as a molecular zipper. The molecular zipper attracts and aligns bio-molecules, or nano-particles along the ridges or valleys. Once the molecules are zipped, nondestructive physical reading is made by the G-ALI applied on a passivation mono-layer graphene which covers the trapped molecules of interest. The G-ALI data are, then, used to identify the molecular structure and/or interaction states, analyzing the graphene atomistics with density functional theory (DFT).