Characterization of Nanostructure Vibration with a Mass-weighted Chemical Elastic Network Model

***Moon K. Kim[1,2], Minhyeok Kim[1], and Soojin Jo[2]**

[1]SKKU Advanced Institute of Nanotechnology, Sungkyunkwan University
[2]School of Mechanical Engineering, Sungkyunkwan University, 440-746 Suwon, Korea

*Corresponding author: mkkim@me.skku.ac.kr

A mass-weighted chemical elastic network model (MWCENM) is introduced as a reliable and effective tool to analyze vibration features of nanostructures including multilayer graphene sheets and artificially synthesized DNA assembly structures. The traditional molecular dynamics simulation and continuum mechanics approach like FEM have both shown difficulty in handling these meso-scale systems due to computational burden and over-simplification, respectively. However, MWCENM is well designed to balance computational efficiency with modeling accuracy by adopting coarse-graining scheme for heavy atoms of interest and also assigning various spring constants based on chemical interaction types. MWCENM successfully revealed frequency shift behaviors of multilayer graphene sheets with respect to the number of layers and stacking order. It was also utilized to predict vibration features (i.e., vibration frequencies and mode shapes) of various DNA hairpin nanostructures designed for biosensors or organic memory devices.

Keywords: Elastic Network Model, Vibration Frequency, Graphene, DNA