Computational Investigation on the pH Sensing Mechanism of Edge-functionalized Graphene Quantum Dots

Bai Anjali, 정용철†
Pusan National University
(greg.chung@pusan.ac.kr†)

Graphene quantum dots (GQDs) have attracted enormous attention as emerging carbon nanomaterials owing to their unique chemical, electronic, and optical properties, which makes them an excellent candidate for bio-imaging, sensing, and photovoltaics. Recent experimental works show that the excitation-dependent emission properties of the GQDs could be tuned based on size, chemical doping, and edge-functionalization, which is critical for a broad range of pH sensing materials. However, the underlying electronic mechanism for pH sensing remains to be poorly understood.
Toward this end, we combined density functional theory (DFT) and time-dependent DFT (TDDFT) calculations to elucidate the underlying pH sensing mechanism for the GQD systems. We carried out large-scale DFT and TD-DFT calculations to evaluate the electronic properties (such as bandgap, pKa, and oscillator strength) of different edge-functionalized GQD structures.