Potential and Versatility of DFT-based Computational Chemistry as an Alternative Research Tool for Chemical Engineers

원용선*
부경대학교
(yswon@pknu.ac.kr*)

With the great advance of computational capacities and softwares, the computational chemistry is now opening a new research perspective to chemical engineers. Here, several inspiring examples using the density functional theory (DFT) calculations are presented and the potential and versatility of computation chemistry in real engineering problems are demonstrated. (1) The design of organic photosensitizer, one of the primary constituents of dye-sensitized solar cells (DSSCs), is discussed. The molecular orbital (MO) structures and absorption properties of organic dyes are computationally obtained by DFT and time dependent DFT (TD-DFT) population analysis and it shows how they are elegantly related to the experimental results. (2) The stabilities of CH4 and SF6 gas hydrate structures arerelatively evaluated based on the calculated binding energies. (3) The catalytic CO2 capture mechanisms in propylene oxide (PO) + KI and PO + KI + glycine systems are proposed in comparison. (4) Initial surface reactions for nucleation during GaN chemical vapor deposition (CVD) are energetically emulated. (5) Some other examples for various applications are presented.