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Manipulation engineering of mechanical properties, band gap, crystal lattice, chemical bonding and optical properties in a novel class of COFs with promising of experimental accessibility

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Covalent-organic frameworks (COFs) constitute an emerging class of porous materials that held together by strong covalent bonds between light elements such as B, C, O, N, H, and Si. COFs display robust thermal stability (400 ~ 600 °C) and have many exotic properties [e.g., high surface areas (as high as 6450 m^2/g), large pore volumes (as high as 5.4 cm^3/g), and the lowest densities for any known crystalline material (as low as 0.17 g/cm^3)]. Even though COFs are in infant stage, they have already demonstrated wide potential applications in various aspects [e.g., gas absorption and storage, catalysis, semiconducting, photo conducting, and optoelectronics,] and great promising for materials science and technology due to their interesting properties. Thus, these materials have attracted ever-increasing attention from different field scientists.

It is still a great challenge to effectively manipulate various properties (especially tailoring the mechanical properties, band gap and optical absorption of COFs with specific targeted applications) with target for the semiconducting COFs, optoelectronics, nanoelectronics, photochemistry at the microscope molecular/atomic level. Here, we for the first time demonstrated that manipulation engineering of a new type of 3D COFs with systematically tunable properties in various aspects (include mechanical properties, band gap, lattice parameter, formation enthalpy, chemical bonding, and optical properties) through detailed DFT calculations. To the best of our knowledge, there is no such attempt on COFs materials so far, the present workrepresent the first comprehensive investigation on systematic tenability of various properties based on our newly proposed manipulation engineering.

Biography

Li-Ming Yang has completed his Ph.D. at the age of 27 years from Jilin University and post doctoral studies from University of Oslo, Norway; Donostia International Physics Center (DIPC), Spain; University of Georgia, Massachusetts Institute of Technology (MIT), USA. Now, he is working in KIST. He has published more than 30 papers in reputed journals (e.g., J. Am. Chem. Soc., Chem. Eur. J., J. Mater. Chem., etc) and has been serving as an invited referee for several journals.

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