Raman Spectra Study and the Corresponding Strain Dependence of Graphyne and Graphdiyne

SHUQING ZHANG, Peking University, COLLEGE OF CHEMISTRY AND MOLECULAR ENGINEERING TEAM — Graphynes, composed of $sp-sp^2$ carbon atoms, have attracted increasing interest of research due to particular optical, electrical and mechanical properties they might have. According to recent theoretical studies prediction, the synthesis of graphyne and graphdiyne are difficult but offer more possible compared to other graphynes, and they have been tried to form and got initial achievement\(^1\). For new materials, their widespread application is impossible without a convinient, fast, non-destructive characterization tool. Raman spectroscopy has performed remarkable ability for studying the properties of $sp^2$ and $sp^3$ carbon materials, such as diamond, graphite, carbon fibers and nanotubes. Naturally, we may expect it is also work in $sp-sp^2$ carbon materials\(^2\). In our work, the Raman features of graphyne and graphdiyne are studied systematically and their variations versus mechanical strain are also investigated by group theory and first-principles calculations. 1. Guoxing Li, et al. Chem. Commun. 2010, 46: 3256 2. Jinying Wang*, Shuqing Zhang*, et al. Phys. Chem. Chem. Phys. 2014, 16 (23): 11303

Shuqing Zhang
Peking University

Date submitted: 05 Nov 2015  
Electronic form version 1.4