

Hybrid triazine-boron two-dimensional covalent organic frameworks : synthesis, characterization, and DFT approach to layer interaction energies.

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Streszczenie

The conversion of 2,4,6-tris(4'-bromophenyl)-1,3,5-triazine to the respective triboronic acid was successfully accomplished by a simple triple Br/Li exchange followed by boronation. Further dehydrative condensation reactions with 2,3,6,7,10,11-hexahydroxytriphenylene or 2,3,6,7-tetrahydroxy-9,10-dilalkylanthracenes (R = Me, Et) resulted in materials featuring good porosity and sorption properties with the nitrogen uptake exceeding 500 cm³/g (STP) and S_{BET} up to 1267 m²/g ($T = 77.2$ K). In addition, simple dehydration of this compound was employed for the preparation of a hybrid 2D COF composed of triazine, boroxine, and benzene rings. The formation of materials was confirmed by the IR analysis and NMR studies on water-decomposed samples. All obtained COFs exhibit high thermal stability with decomposition temperatures in the range of 400–600 °C. They also show quite different morphology ranging from regular 0.5–4 μm spherical and ellipsoidal clusters to 5–12 μm bent rodlike particles. The PXRD studies supported by periodic DFT modeling in Crystal09 package revealed the formation of crystalline 2D honeycomb-type lattices with eclipsed stacking models. In addition, the differences between boroxine-triazine material and related COF-1 and CTF-1 structures were investigated by comparing layer interaction energies, work function values as well as atomic charges and electrostatic potential maps plotted on the electron density surfaces. It demonstrates that the interactions between layers are enhanced by the stacking of triazine and boroxine rings. Finally, we have investigated the upper limit to space accessible volume using a procrystal electron density approach.

Słowa kluczowe

covalent-organic frameworks, two-dimensional materials, adsorption, periodic DFT calculations, interlayer energy, layer assembly, boron-triazine COFs

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