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Visible-light absorption in 2D covalent triazine framework: enhanced by interlayer coupling and pore size increasing XUE JIANG, JIJUN ZHAO, Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Dalian University of Technology), Ministry of Education,Dalian 116024,China, DALIAN UNIVERSITY OF TECHNOLOGY COLLABORATION — Compared with traditional bulk materials, two-dimensional (2D) crystals have some intrinsic advantages as photocatalysis owing to the limited thickness and large surface area. So far, many monolayer materials have been shown to be potential photocatalysis for water splitting from both theoretical calculations and experiments; while most of them are inorganic materials. In contrast, g-carbon nitride, as a starting successful case, motivates us to explore 2D organic semiconductors, which have not yet well investigated. Using first principles calculations, we predicted a family of 2D covalent triazine framework (CTF) as a promising visible-light-driven photocatalyst by studying their electronic structures, work function, CBM/VBM position, and optical absorption spectra. Moreover, we found that multilayer CTF have much better visible-light adsorption than a single layer induced by the interlayer coupling. In addition, controlled construction of such CTF from suitable organic subunit pave the way for connection between the optical energy gap of CTF and pore size. The insights from our study not only enrich the family of organic semiconductor photocatalyst, but also are very helpful in designing and assembling CTF subunits for optimal performance.

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