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Heptagon-Azulene Embedded Helical Bilayer Nanographene

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Twisted bilayer graphene and related nanographens exhibit outstanding electronic and physical properties [1]. However, the synthesis of structurally well-defined and defect bilayer nanographenes is still challenging. Here, a unique non-hexagonal helical bilayer nanographene has been synthesized. The heptagon and azulene embedded bilayer molecule represents the first non-hexagonal π−extended [10]helicene with a total of 35 fused rings. The folded bilayer structure was investigated theoretically and confirmed by single-crystal x-ray diffraction, revealing a highly twisted conformation and strong π−π interactions between the two layers. The enantiomers were separated, and their chiroptical properties were evaluated, showing the ECD responses of this novel chiral bilayer nanographenes. This non-hexagonal helical bilayer nanographene (**NHBNG**) could potentially serve as a seed for the preparation of structurally well-defined bilayer nanographene.

References

[1] Nimbalkar, A.; Kim, H. Opportunities and Challenges in Twisted Bilayer Graphene: A Review. Nano-Micro Letters, 12(2020), 126.

Figures

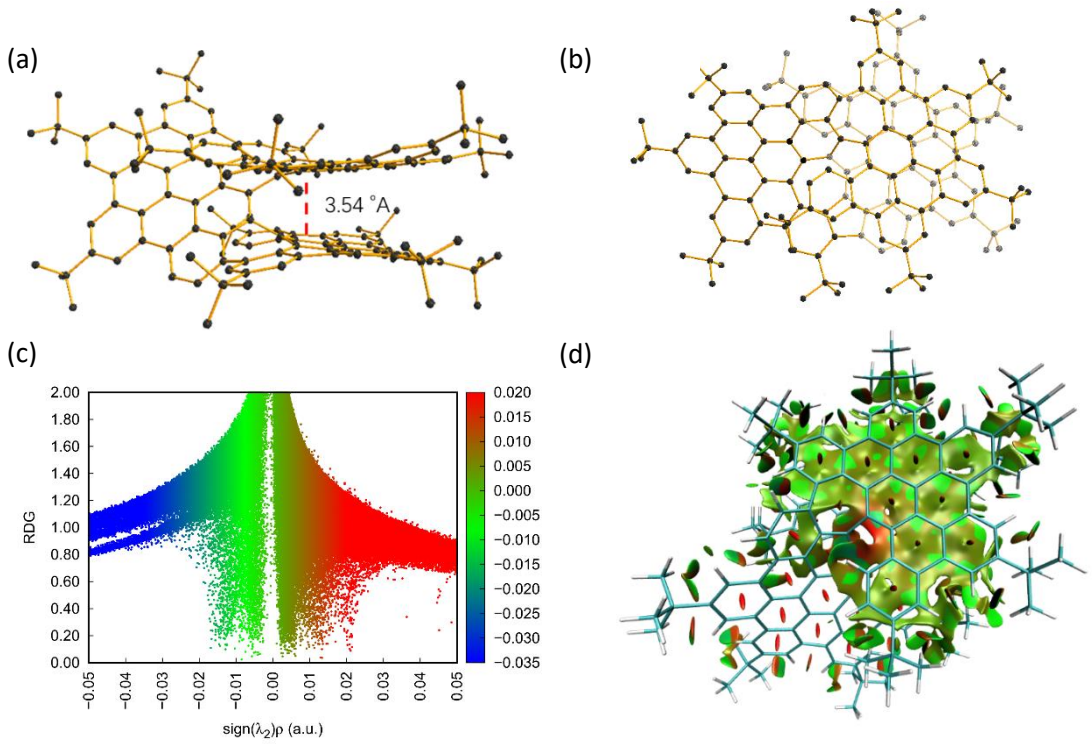

Figure 1: (a) side and (b) top view of **NHBNG 1**. The thermal ellipsoids are set at a probability level of 50%. (c) Graphical representation of the reduced density gradient(RDG) versus sign(λ2)ρ, in which the blue, green, and red color of the vertical scale represent the hydrogen bonding, Vandel Walls effect, and steric effect, respectively. (d) Plots of the reduced density gradient isosurfaces for compound **NHBNG 1**.