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Heptagon-Azulene Embedded Helical Bilayer Nanographene

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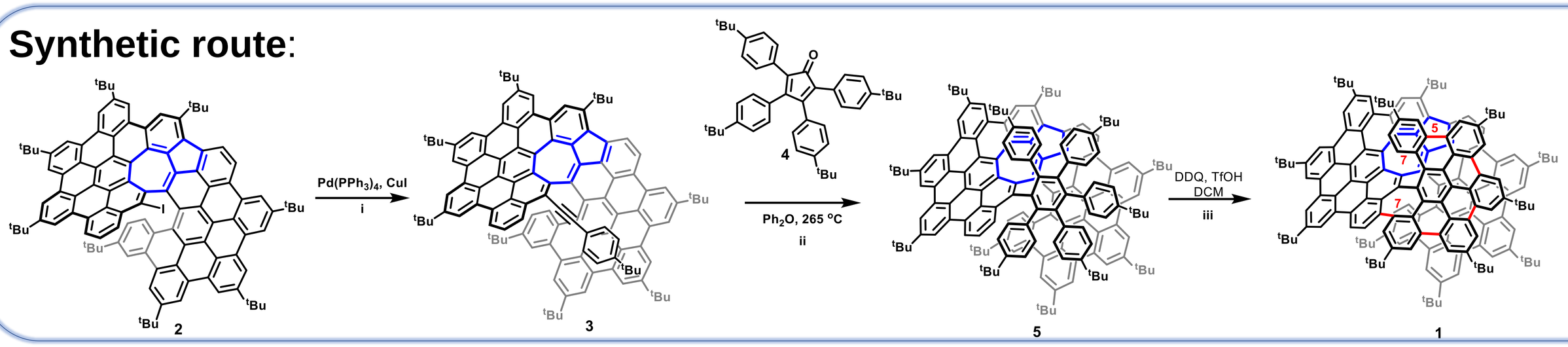
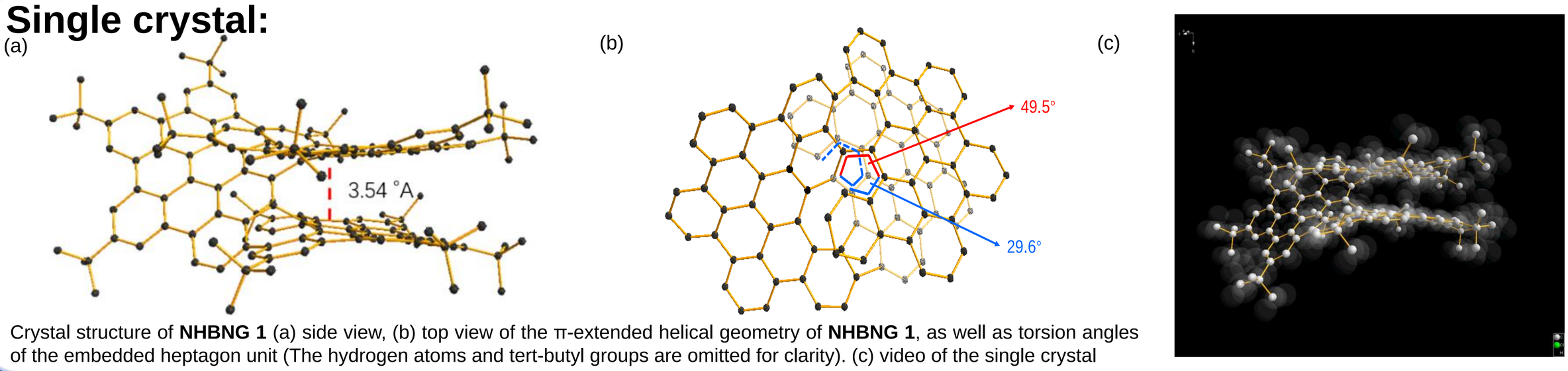
Introduction: Twisted bilayer graphene and related nanographens exhibit outstanding electronic and physical properties[1]. However, the synthesis of structurally well-defined and defect bilayer nanographenes is still missing. Here, a unique non-hexagonal helical bilayer nanographene (NHBNG) has been synthesized. The heptagon and azulene embedded bilayer molecule represents the first non-hexagonal π−extended [10]helicene with a total of 35 fused rings.

Synthetic route:

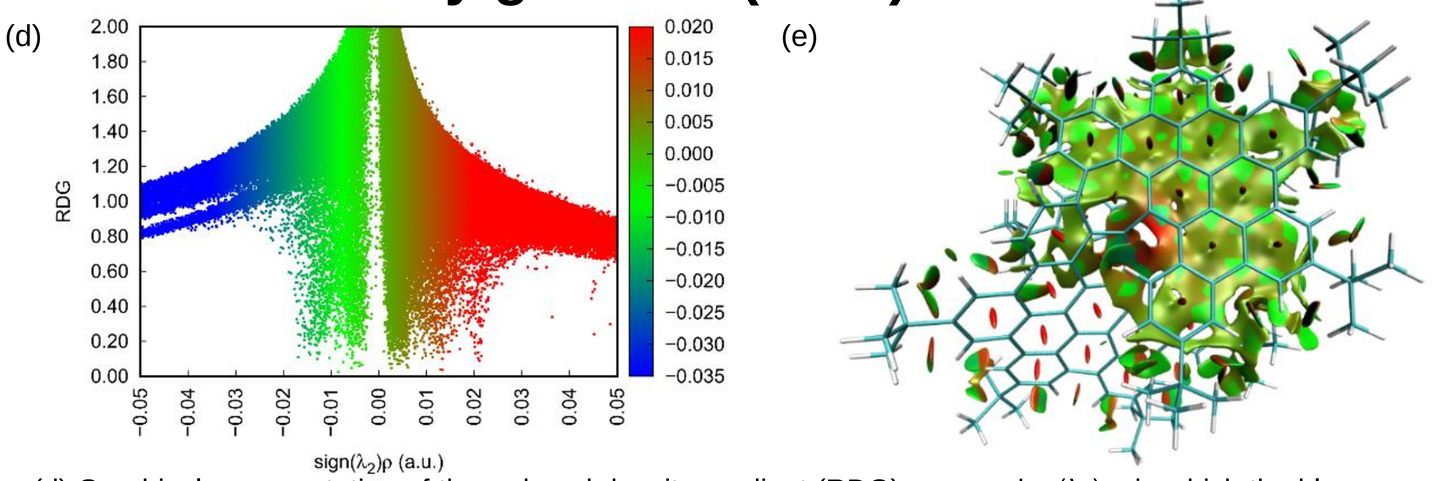


Single crystal:



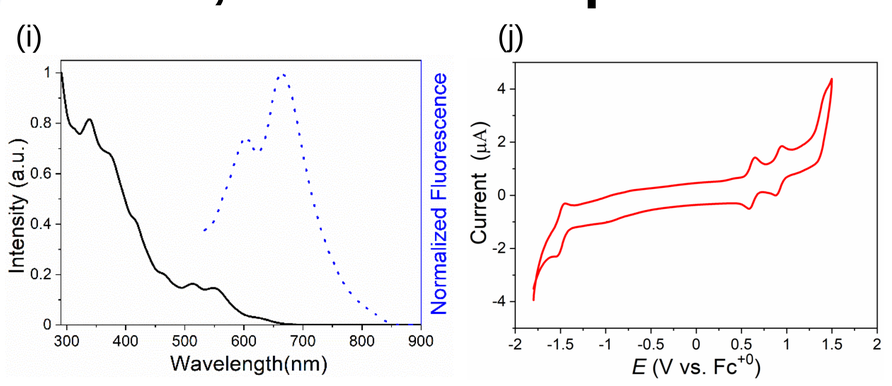
Crystal structure of **NHBNG 1** (a) side view, (b) top view of the π-extended helical geometry of **NHBNG 1**, as well as torsion angles of the embedded heptagon unit (The hydrogen atoms and tert-butyl groups are omitted for clarity). (c) video of the single crystal

Reduced density gradient (RDG):



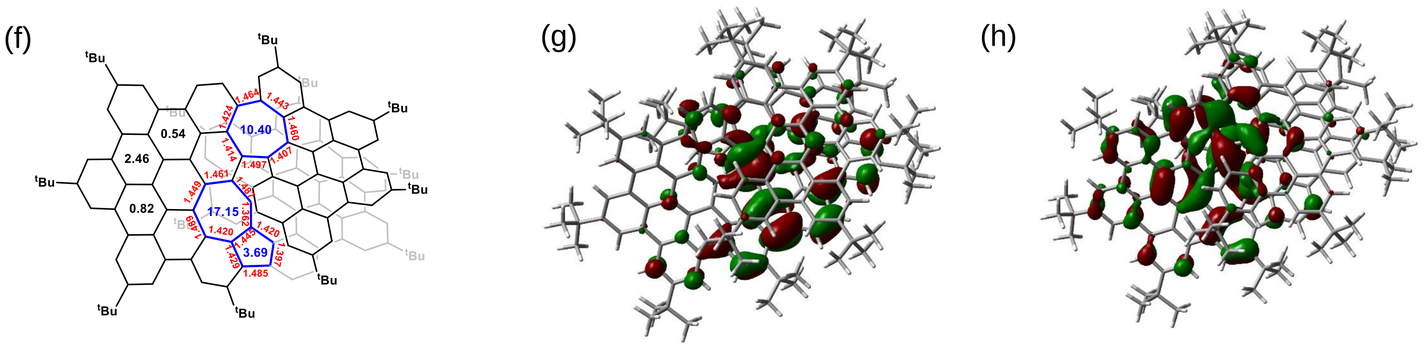
(d) Graphical representation of the reduced density gradient (RDG) versus sign(λ_2)ρ, in which the blue, green, and red color of the vertical scale represent the hydrogen bonding, Van der Walls effect and steric effect, respectively. (e) Plots of the reduced density gradient isosurfaces for compound **NHBNG 1**.

UV/Vis, PL and CV spectra:



(I) UV-vis absorption (black line) and photoluminescence emission (PL, dashed blue line, excitation at 510nm) spectra of **NHBNG 1** in CH_2Cl_2 (1×10^{-5} mol/L). (j) Cyclic voltammetry (CV) of c in CH_2Cl_2 containing 0.1 M nBu$_4$NPF$_6$ at a scan rate of 50 mVs^{-1} at room temperature.

NICS and HOMO/LUMO calculations:



(f) Nucleus independent chemical shift calculations (NICS(1)) values (blue/black) of **NHBNG 1**, calculated at the GIAO-B3LYP/6-31+G(2d,p) level of theory, as well as the bond lengths (red, in Å) of the embedded heptagon-azulene units. Frontier molecular orbitals of **NHBNG 1** (g) HOMO (h) LUMO. The calculations were performed at the B3LYP 6-31G (d) level.

Outlook:

This non-hexagonal helical bilayer nanographene (NHBNG) could potentially serve as a seed for the preparation of structurally well-defined bilayer nanographene. It encourages us to design and synthesize non-hexagon superhelicenes and multilayer nanographenes.

Reference: *Nano-Micro Letters*, **2020**, *12*, 126