Supporting Information

Phase Transition from a Nonmagnetic to a Ferromagnetic State in a Twisted Bilayer Graphene Nanoflex: The Role of Electronic Pressure on the Magic-Twist

Dharmendra Pant[1] and Ranjit Pati[1,2]*

[1]*Department of Physics, Michigan Technological University, Houghton, MI 49931, USA*

[2]*Henes Center for Quantum Phenomena, Michigan Technological University, Houghton, Michigan 49931, USA.*

*Corresponding author. Email: patir@mtu.edu

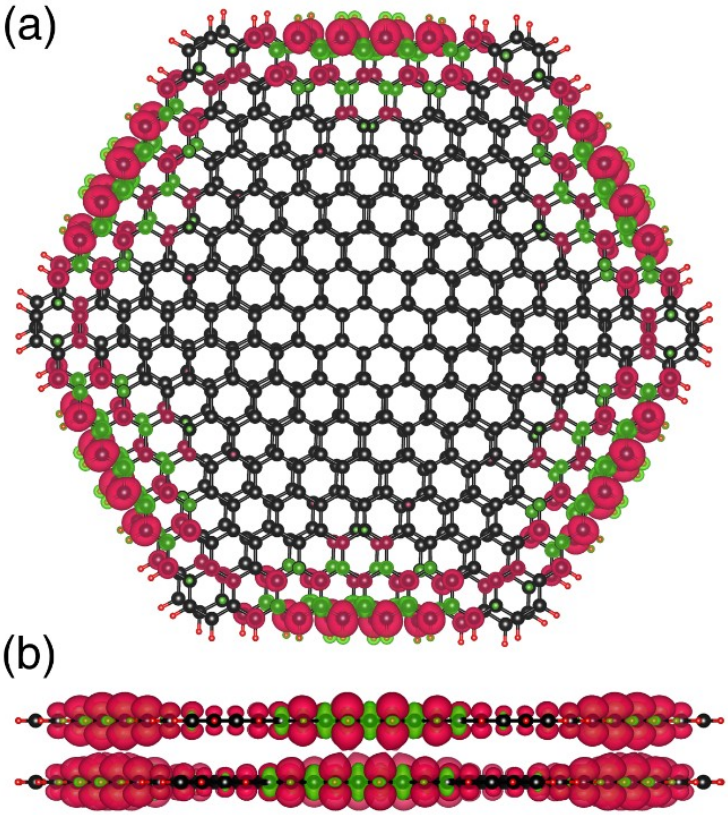

Figure S1. Magnetization density in a twisted bilayer graphene nanoflex at P_e = -0.042 GPa (θ_M = 2.4°). (a) Top view, **(b)** Side view of the magnetization density obtained using DFT with the PBE form of exchange-correlational functional. The red color represents the spin-up states, while the green color represents the spin-down states. The p-orbitals at the boundary contribute to magnetism.

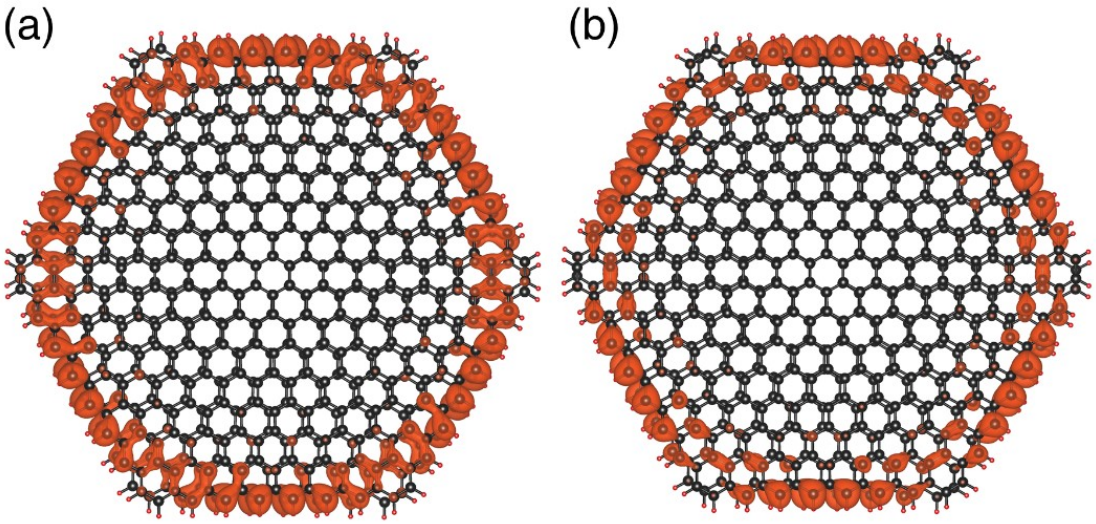

Figure S2. Unstable frontier electronic states in a twisted bilayer graphene nanoflex at P_e = -0.042 GPa (θ_M = 2.4°). (a) Highest Occupied and **(b)** Lowest Unoccupied orbitals are isomorphic and nearly energy degenerate.

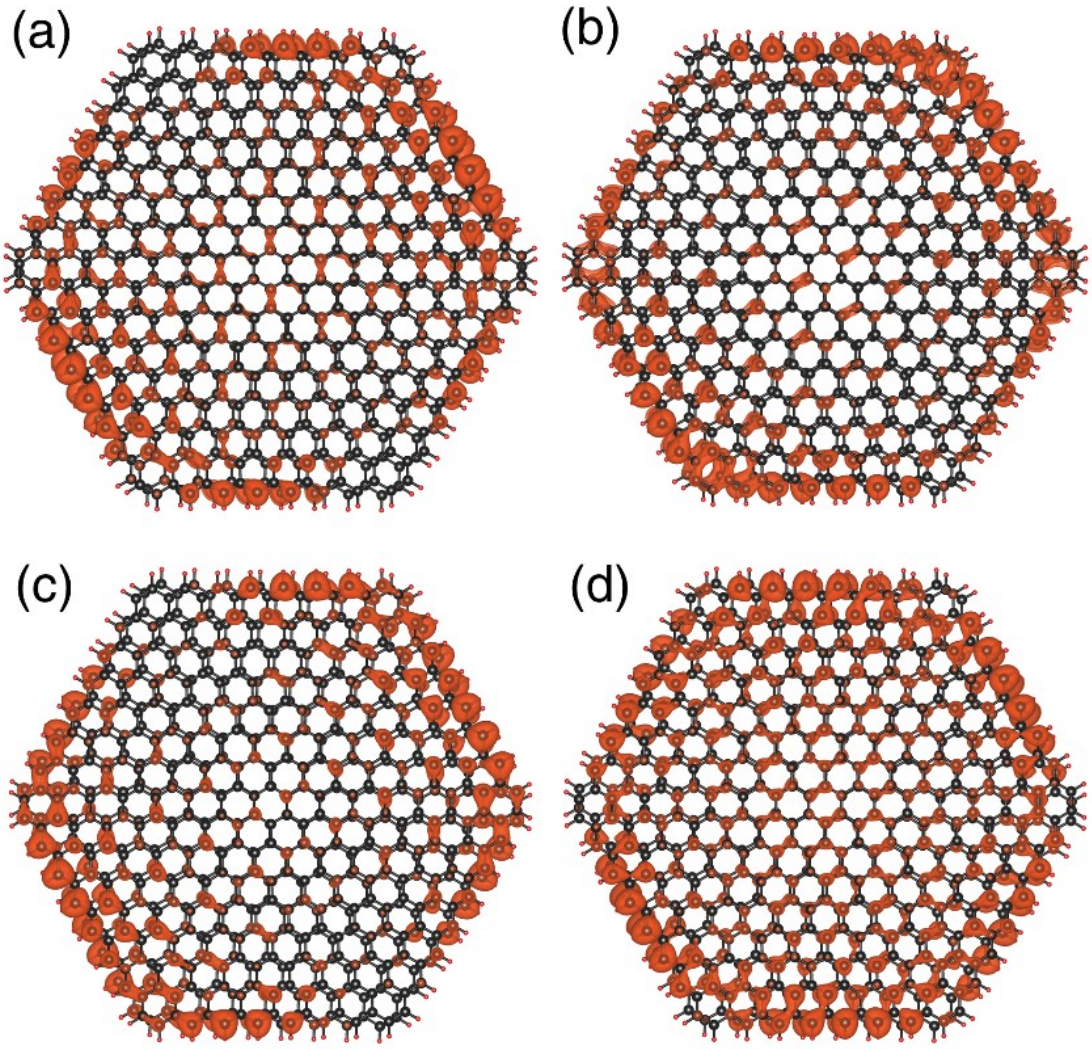

Figure S3. Stable broken symmetry ferromagnetic gap states in a twisted bilayer graphene nanoflex at P_e = -0.042 GPa (θ_M = 2.4°). (a) Highest Occupied (HO) state for the spin-majority (α) electrons, **(b)** Lowest Unoccupied (LU) state for the α electrons, **(c)** HO state for the spin-minority (β) electrons, and **(d)** LU state for the β electrons.

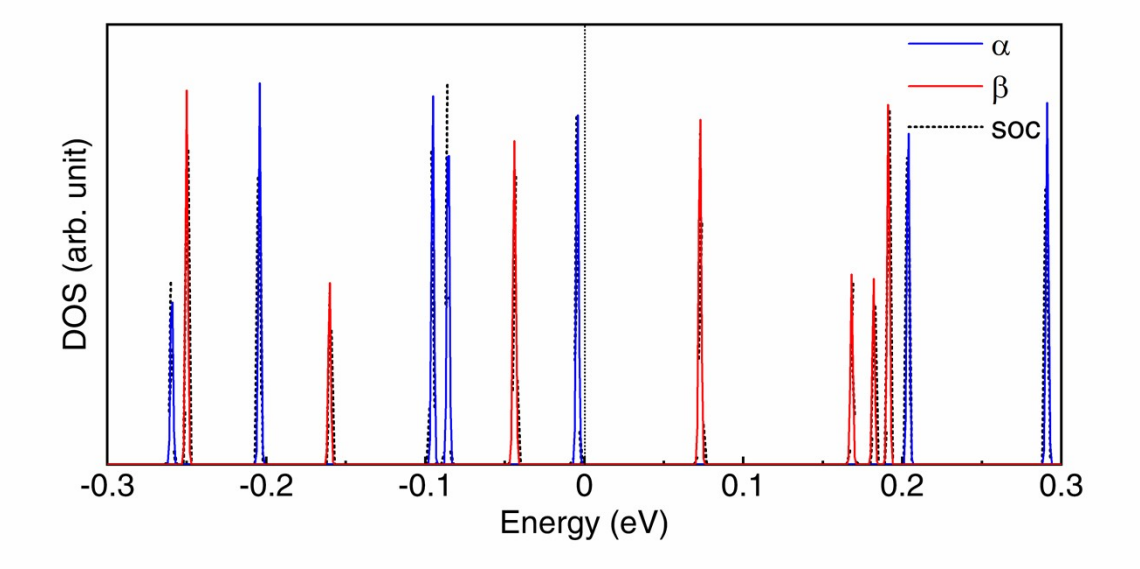

Figure S4. Density of states in a twisted bilayer graphene nanoflex at P_e = -0.042 GPa (θ_M = 2.4°) with and without spin-orbit coupling. The inclusion of spin-orbit coupling does not show any significant shift in the energy spectrum obtained using DFT with PBE exchange-correlation functional.