Electronic Supplementary Information

Interlayer electron flow and field shielding in twisted trilayer graphene quantum dots

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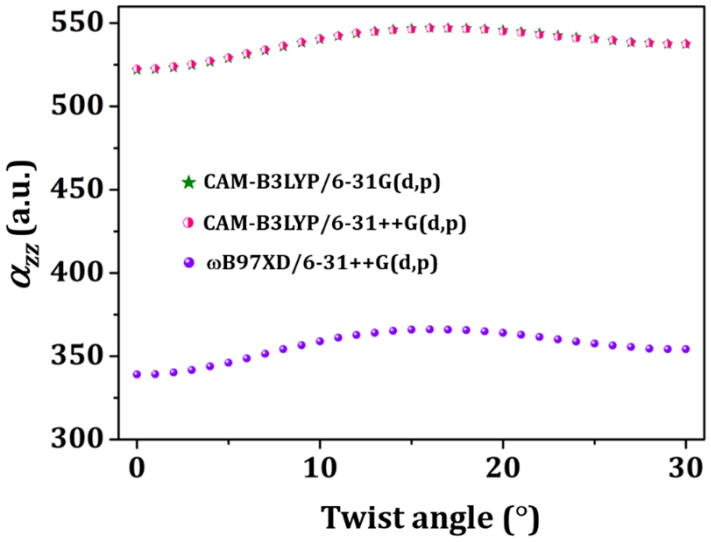

Figure S1. The computed α_{zz} values with the CAM-B3LYP and ωB97XD functionals and the 6-31G(d,p) and 6-31++G(d,p) basis sets.

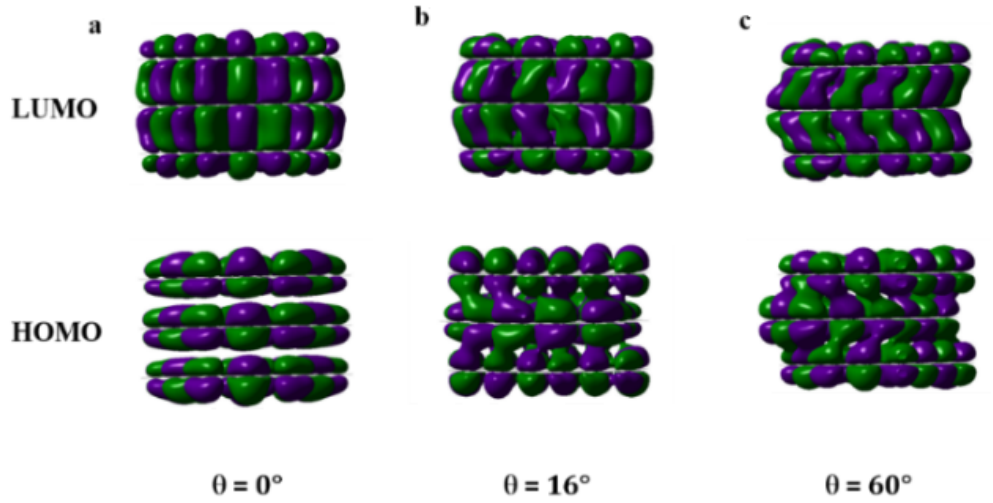

Figure S2. HOMO and LUMO in RFR with an isovalue of 0.005 a.u. at θ = 0° (a), 16° (b) and 60° (c), respectively.

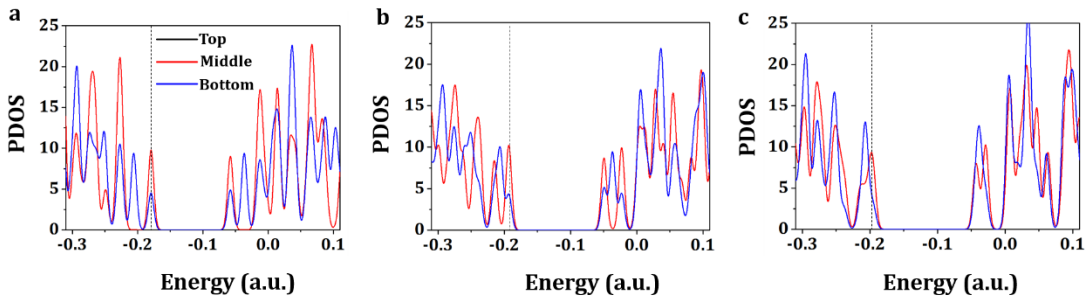

Figure S3. PDOS of the top, middle and bottom layers of RFR rotating about the C atom of the innermost shell at $\theta = 0°$ (a), 16° (b) and 60° (c), respectively. The black and blue lines are coincident with each other. The HOMO is marked by dotted line.

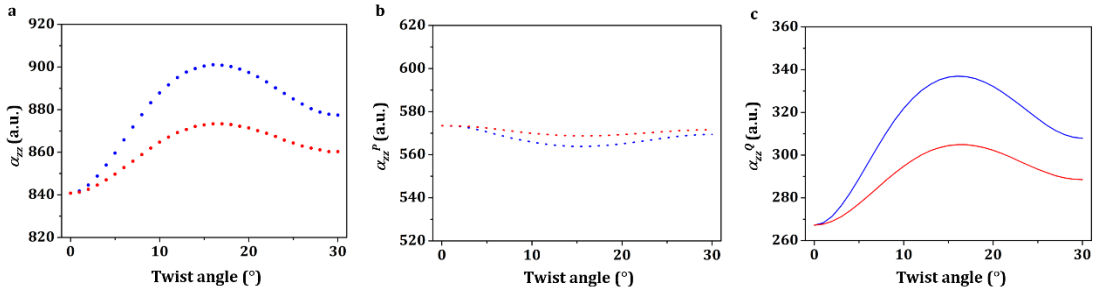

Figure S4. The polarizability (α_{zz}, a) and its dipole ($\alpha_{zz}{}^{P}$, b) and CT ($\alpha_{z}{}^{Q}$, c) parts of the RFR (in blue) and FRR (in red) structures rotating about R_{II}.

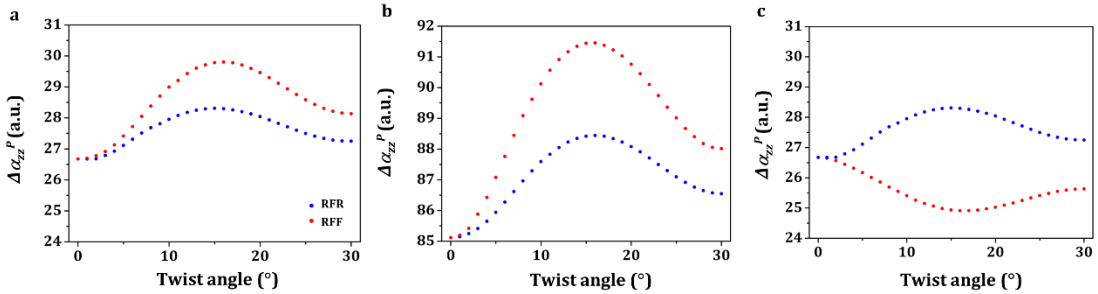

Figure S5. The variation in dipole polarizability ($\Delta\alpha_{zz}^{P} = \alpha_{0,zz} - \alpha_{zz}^{P}$) of the top (a), middle (b) and bottom (c) layers of the RFR and FRR structures rotating about R_{II}. $\alpha_{0,zz}$ = 237.3 a.u. is the polarizability component of the corresponding monolayer.

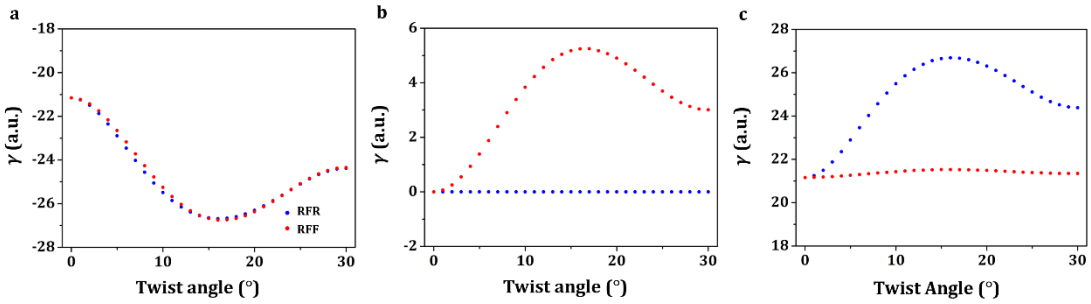

Figure S6. Total dq/dF (γ) of the bottom (a), middle (b) and top (c) layers of RFR and RFF structures rotating about R_{II}, respectively.

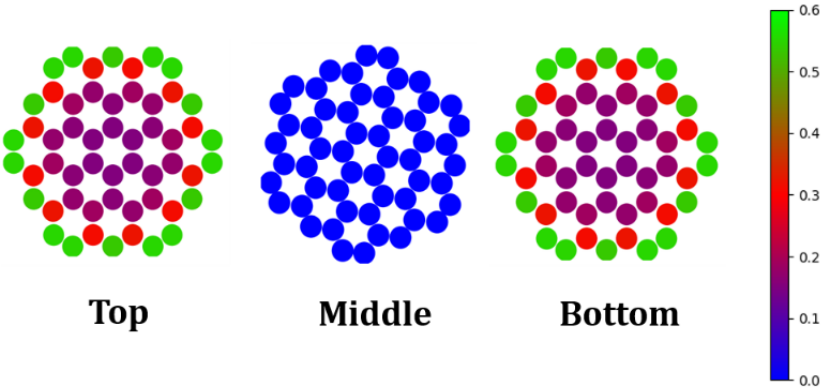

Figure S7. Atomic γ (in absolute value and in a.u.) in the top, middle and bottom layers of the RFR structure rotating about R_{II} at $\theta = 16°$, respectively.

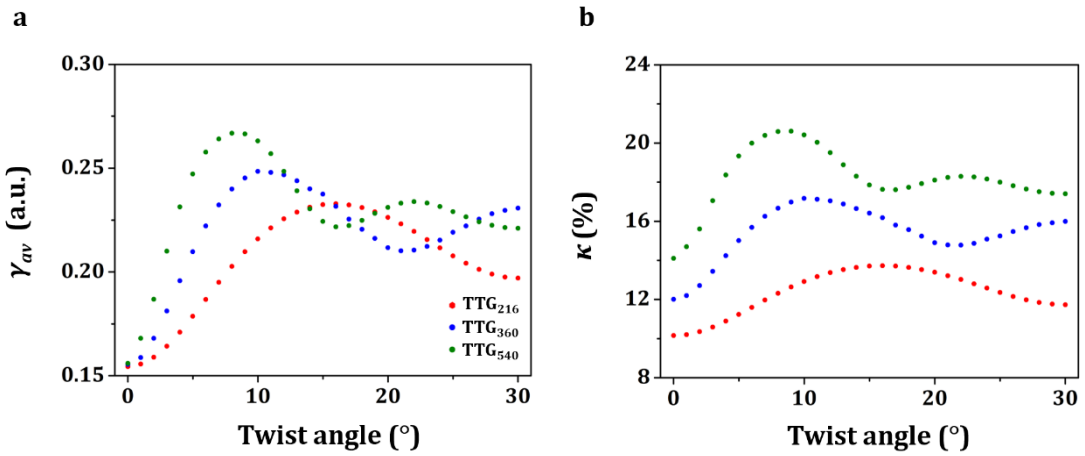

Figure S8. Computed averaged γ_{av} (a) and κ (b) for the structures rotating about R_{II}. N is the number of atoms in the QD.