Controllable interlayer shielding effect in twisted multilayer graphene quantum dots

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Fig. S1 HOMO and LUMO in TMG_{72,2} with an isovalue of 0.005 a.u. at $\theta = 0^{\circ}$ (a), 16° (b) and 58° (c), respectively. Orbital overlap between the upper and lower layers is not found in the HOMO of the structure of $\theta = 0^{\circ}$, but found in the structures of $\theta = 16^{\circ}$ and 58°. Fig. S2 Total density of states (TDOS) of TMG_{72,2} of $\theta = 0^{\circ}$, 16° and 58°.

Fig. S3 Changes in dipole polarizability $(\Delta \alpha_{zz}^{P} = \alpha_{zz}^{P} - \alpha_{zz}^{0})$ of layers in TMG_{72, N} (N = 2–10) versus twist angle by taking the polarizability component of monomer ($\alpha_{zz}^{0} = 143.8$ a.u.) as a reference.

Fig. S4 The relationship between interlayer distance and rotational modes regarding $\bar{\alpha}_{zz}$. (a) Model I and (b) Model II.

Fig. S5 (a) The averaged axial polarizability of $TMG_{36, N}$ (N = 1-12) and (b) $TMG_{120, N}$ (N = 1-6) at a varying twist angle.

Table S1 The absorption wavelength (λ , nm), and transition dipole moment (μ_{ij} , a.u.) between the ground state and excited states corresponding to the first prominent peaks in absorption spectra of TMG_{72,2} in Fig. 3.



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|------------------------------------|--------------|--------------|--------------|-----|--------------|
| spectra of $TMG_{72,2}$ in Fig. 3. | | | | | |
| θ | $\mu_{ij,x}$ | $\mu_{ij,y}$ | $\mu_{ij,z}$ | λ | $ \mu_{ij} $ |
| 0° | -0.295 | -0.006 | 0.000 | 395 | 0.295 |
| 16° | 0.000 | -0.830 | 0.000 | 480 | 0.830 |
| 58° | -0.436 | 0.000 | 0.526 | 472 | 0.683 |

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