Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.


# Supporting Information

**Computational Method (PWmat)**

Additional relaxation and DOS calculations for PbS QDs were conducted using the plane-wave basis set software PWmat. Within the GGA framework of the PBE functional, all calculations employed the PD04 norm-conserving pseudopotential, with a cutoff energy set to 50 Ry. The energy convergence criteria for atomic forces and self-consistent calculations were consistent with those in the main text. Due to the sufficiently large computational system (197 atoms), only a single Γ-point sampling was considered.

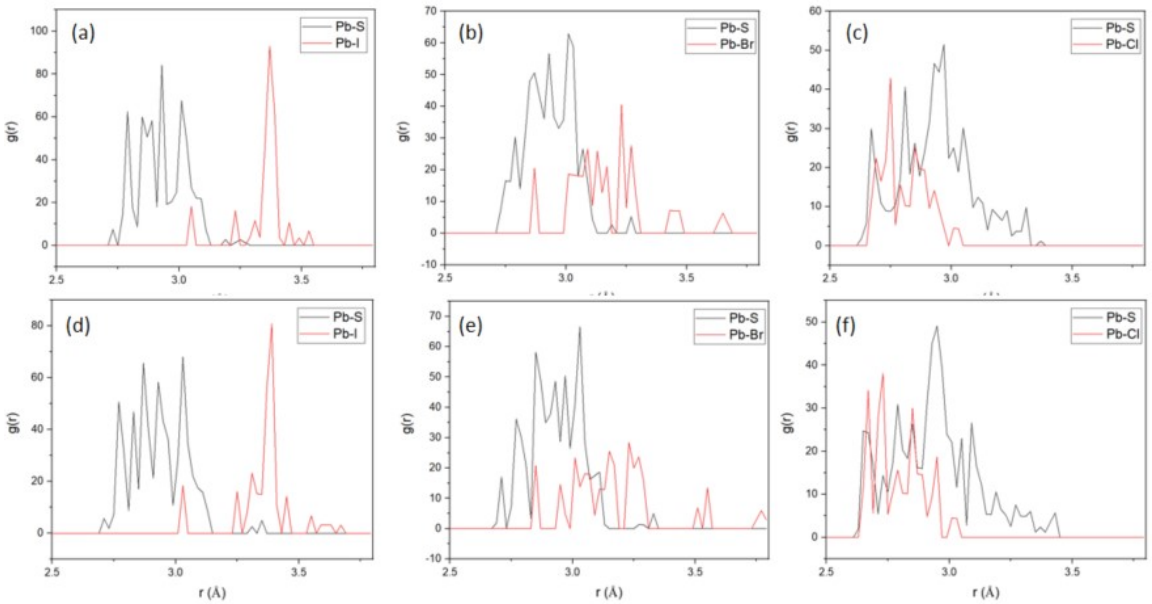


Figure S1. Radial distribution functions of three types of PbS QDs optimized using OpenMX (a), (b), (c), and PWmat (d), (e), (f).

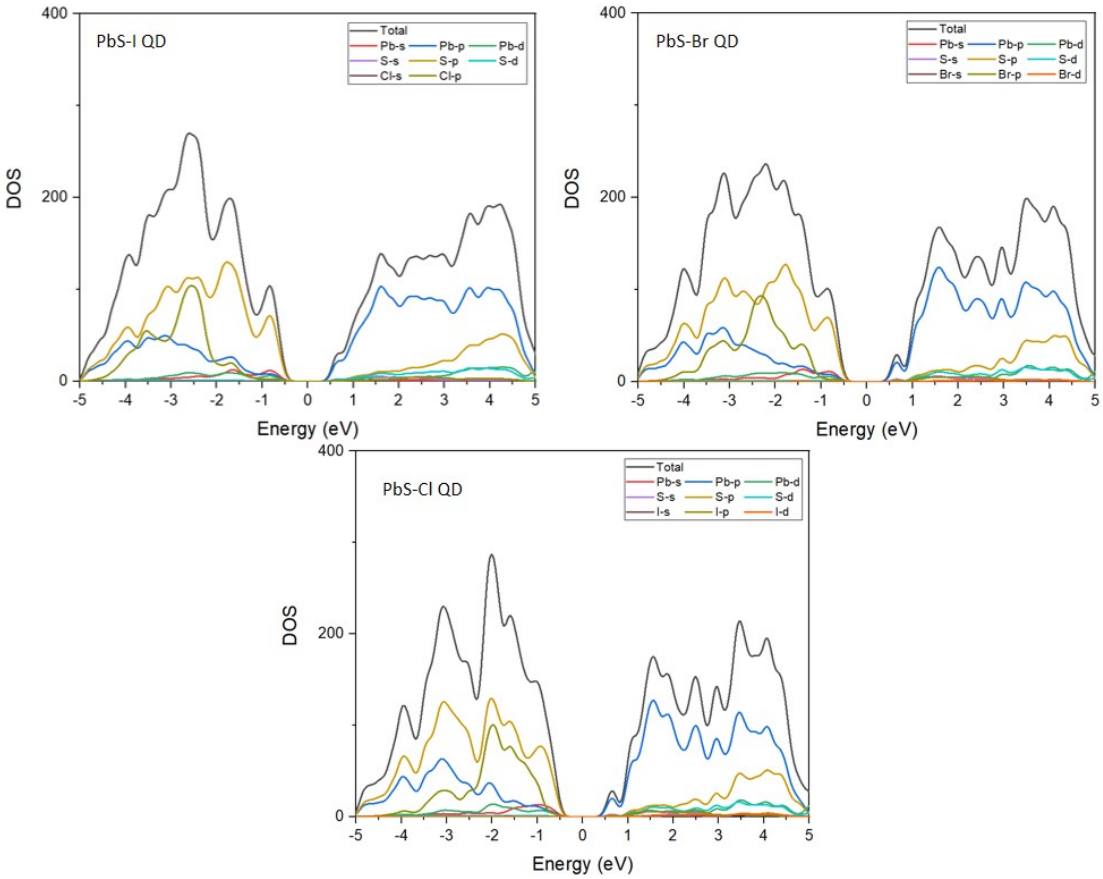


Figure S2. Atomic orbital projected density of states for three types of PbS quantum dots.

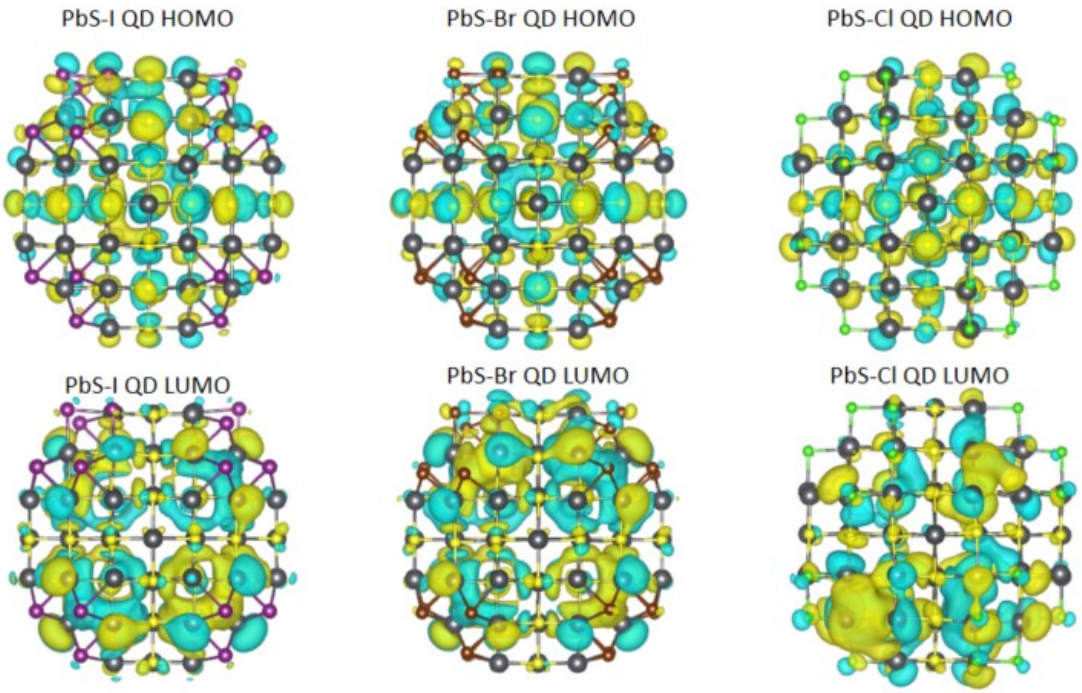


Figure S3. Wave functions of HOMO and LUMO for the three types of PbS QDs.

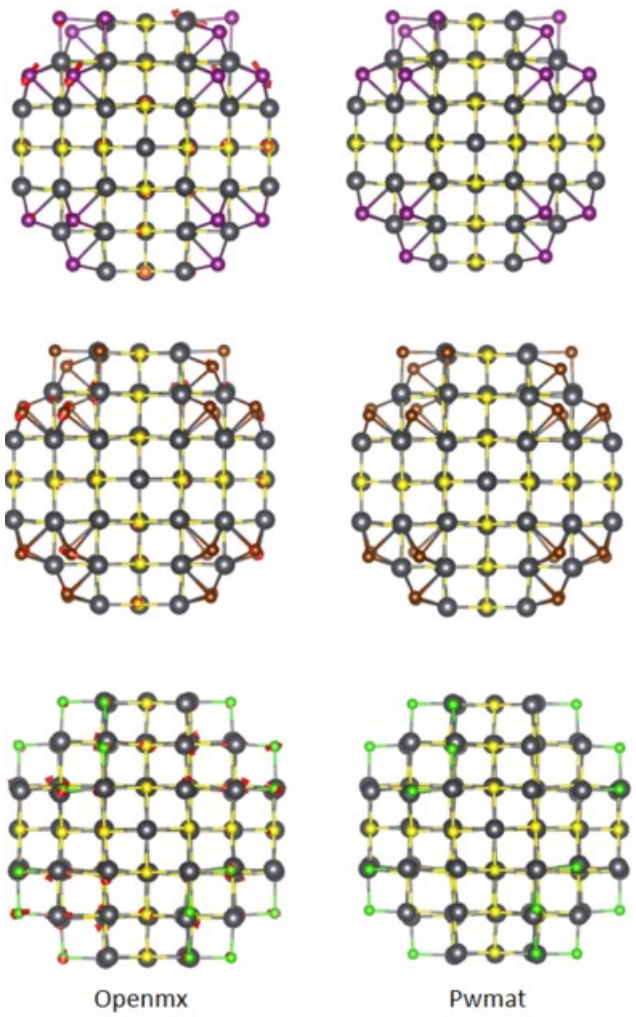


Figure S4. Structures of the three types of PbS QDs optimized using Openmx and PWmat Code. Red vectors corresponding to the deviation of atomic coordinates in optimized structures.

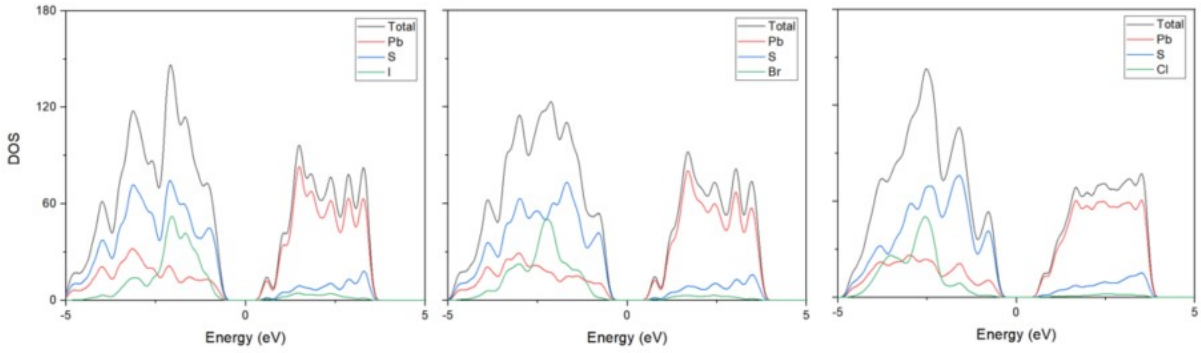


Figure S5. DOS and PDOS for the three types of PbS QDs calculated using PWmat.

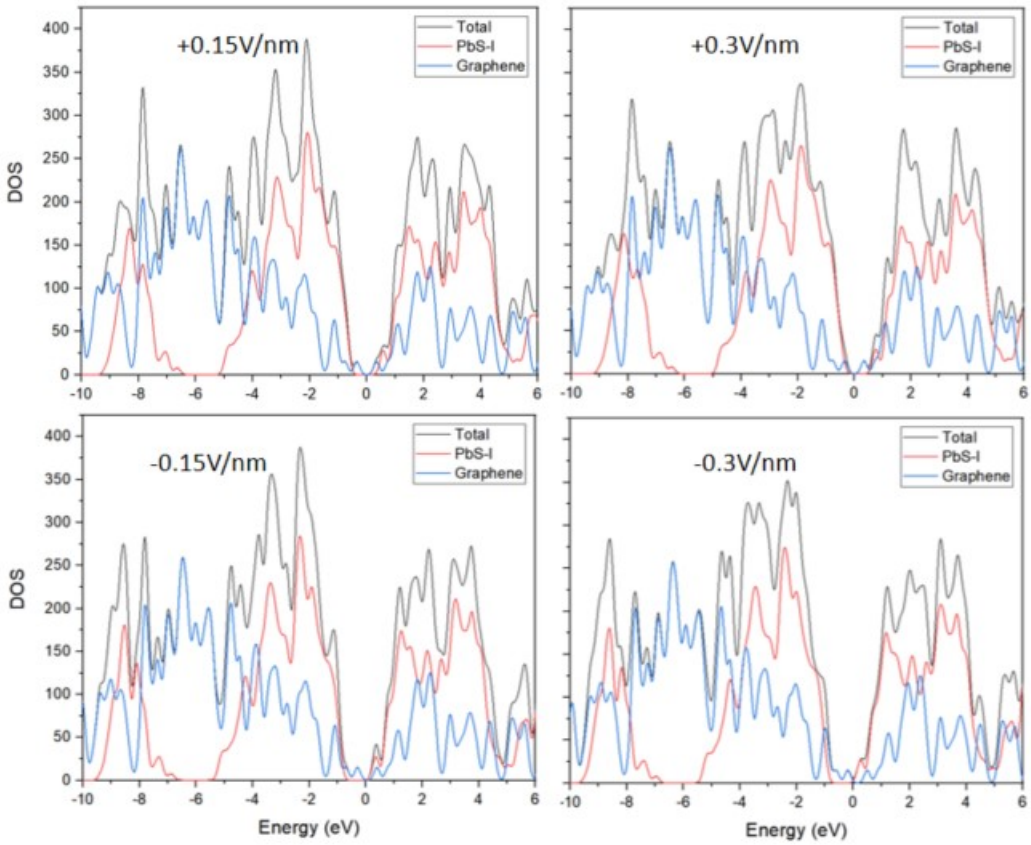


Figure S6. DOS and PDOS of the PbS-I QD/graphene system under ±0.15 and ±0.3V/nm electric field strengths.

Table S1. Root mean square deviation(RMSD) of the three types of PbS QDs optimized using OpenMX and PWmat.

| System | RMSD (Å) |
|---|---|
| PbS-I QD | 0.043 |
| PbS-Br QD | 0.030 |
| PbS-Cl QD | 0.049 |