Supplementary materials

**Photoluminescence enhancement assisted by the surface state emission of** [**aluminum**](javascript:;) **ion intercalated MoS2 quantum dots**

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FIG. S1. (a) TEM image of uniformly dispersed pristine MoS2 QDs, and the inset is HRTEM image of a single MoS2 QD which shows the lattice spacing. (b) The corresponding size distribution histograms of MoS2 QDs shown in (a). The size was statistically calculated from 200 dots randomly selected and measured. (c) AFM image of MoS2 QDs deposited on freshly cleaved mica substrate. (d) The corresponding line profile indicated by the green line in (c).



FIG. S2: Atomic structures and electronic densities of states (DOS) of pristine and Al-adsorbed MoS2 nanoribbons. (a) Atomic structure of pristine MoS2 nanoribbon, (b) Atomic structure of Al-adsorbed MoS2 nanoribbon, and the top (up) and side (bottom) views of the atomic structure are shown. The electronic DOS of pristine and Al-adsorbed MoS2 nanoribbons and projected DOS (PDOS) of Al-3*p* and S-3*p* in Al-adsorbed MoS2 nanoribbon are provided in (c), respectively. Large (purple and blue) and medium (yellow) balls are Mo, Al, and S atoms, respectively. The zero of energy is set at the Fermi level shown by dash-dotted dark lines. Densities of states with blue and red lines show spin-up and spin-down states, respectively.

Density functional theory (DFT) calculations: Our DFT calculations have been performed using projector augmented wave (PAW) potentials as implemented in the Vienna Ab initio Simulation Package (VASP). The exchange correlation potential is approximated by generalized gradient approximation (GGA) using PBE functional for spin-polarized calculations of pristine and Al-adsorbed MoS2 nanoribbons. The kinetic cutoff energy for the plane wave expansion was set to 450 eV. A vacuum layer of 15 Å was used to prevent periodic image interactions. The convergence for energy is chosen as 10-4 eV between two consecutive steps, and the maximum Hellmann-Feynman forces acting on each atom is less than 0.03 eV/Å upon ionic relaxation. The K-point sampling in the Brillouin zone was carried out by the Monkhorst-Pack scheme with the grids of 9×1×1 k-points for the pristine and Al-adsorbed MoS2 nanoribbons.

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FIG. S3. Photoluminescence spectra of MoS2 QDs prepared with and without metal ions under excitation wavelength at 350 nm.

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FIG. S4. (a) and (b) UV–Vis absorption and PL spectra of MoS2 QDs in DMF solutions with different concentration.

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FIG. S5. Photoluminescence spectra of pristine MoS2 QDs with and without Al3+ ions under excitation wavelength at 350 nm.

Table SI. Biexponential fitting for time-resolved PL spectra of the MoS2 QDs at detection wavelength of 410 nm when excited at 340, 350, and 370 nm.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ex | A1 | A2 | τ1(ns) | τ2(ns) |
| 340 nm | 77% | 23% | 1.70 | 8.01 |
| 350 nm | 78% | 22% | 1.69 | 8.01 |
| 370 nm | 84% | 16% | 1.68 | 8.01 |