Supporting Information

Rapid Exfoliation of Layered Covalent Triazine-based Frameworks into N-Doped Quantum Dots for Selective Detection of Hg^{2+} Ions

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Computational Methods

DFT computations were performed using the plane-wave technique implemented in Vienna *ab initio* simulation package (VASP).[1] The ion-electron interaction was described using the projector-augmented plane wave (PAW) approach.[2] The generalized gradient approximation (GGA) expressed by PBE functional[3] and a 500 eV cutoff for the plane-wave basis set were adopted for geometry optimizations. As PBE method systematically underestimates the band gaps of semiconducting materials, we thus utilized the HSE06 hybrid functional[4] for the computations of electronic and optical properties. The convergence threshold was set as 10^{-4} eV in energy and 10^{-3} eV/Å in force. We set the *x* and *y* directions parallel and the *z* direction perpendicular to the layer plane, and adopted a supercell length of 15 Å in the *z* direction. The Brillouin zones was sampled with a 5×5×1 Γ centered *k* points grid. To given an intuitive demonstration of the optical properties, we also computed the imaginary part of the dielectric function (ε_2) of CTF-1 according to the following equation:[5]

$$\varepsilon_2(\omega) = \frac{4\pi^2 e^2}{\Omega} \lim_{q\to 0} \frac{1}{q^2} \sum_{c,v,\vec{k}} 2w_{\vec{k}} \delta(\varepsilon_{c\vec{k}} - \varepsilon_{v\vec{k}} - \omega) \times \left\langle \mu_{c\vec{k}+e_\alpha \vec{q}} \middle| \mu_{v\vec{k}} \right\rangle \left\langle \mu_{c\vec{k}+e_\beta \vec{q}} \middle| \mu_{v\vec{k}} \right\rangle^*$$

where the indices *c* and *v* refer to the conduction and valence band states, respectively, and μ_{ck} is the cell periodic part of the orbits at the k-point.

Supplemental Experimental results

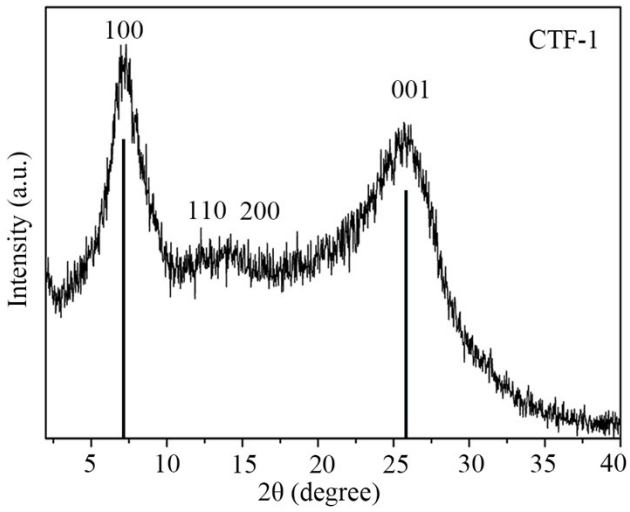

Figure S1| XRD of CTF-1. The low angle peak (∼7°) could be interpreted as the in-plane reflection (100) of the ideal 2D porous-honeycomb structure consist of benzene rings and triazine, while the broad (001) diffraction peak at ∼26° could be attributed to a vertical spacing between stacked sheets of 3.4 Å.

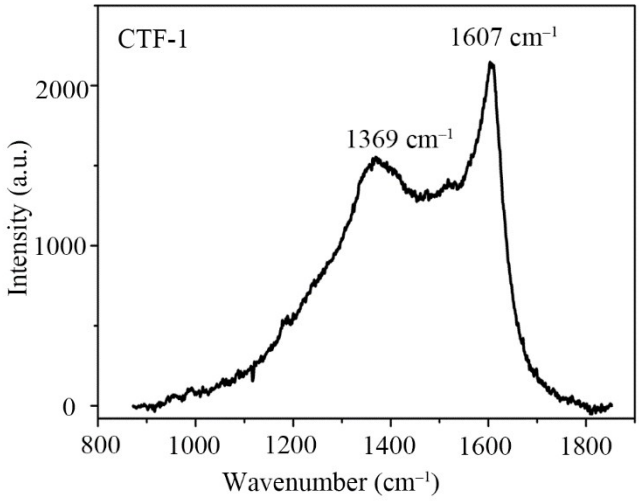

Figure S2| Raman spectra of the CTF-1 at a laser excitation of 433 nm. The G band at 1607 cm^{-1} reveals the existence of extend π-conjugation and the D band at 1369 cm^{-1} is attributed to the structure disorder.

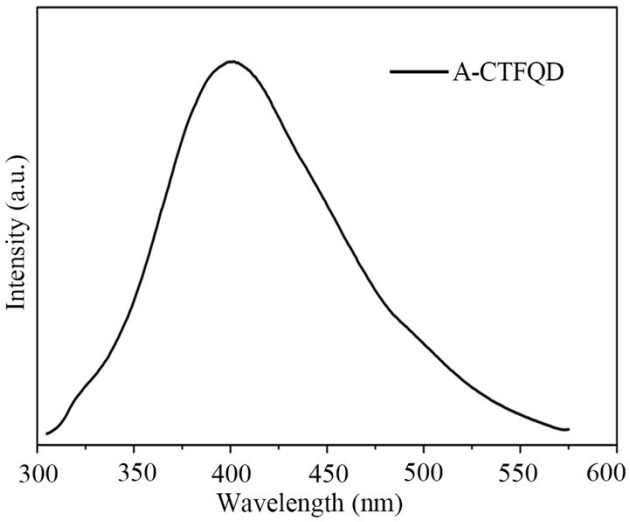

Figure S3| The PL spectra of A-CTFQD excited at 290 nm.

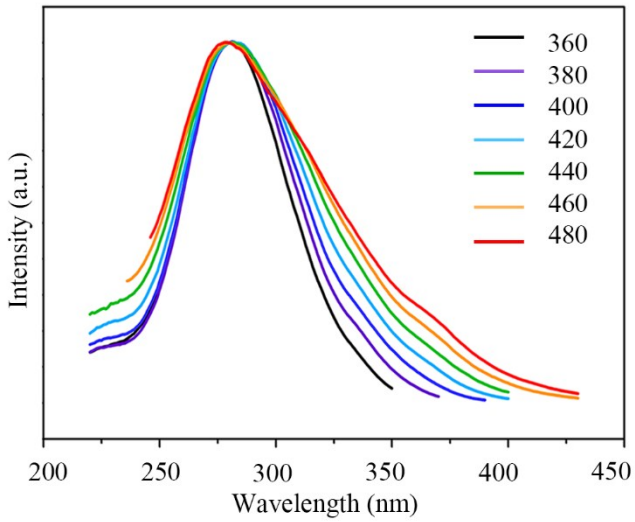

Figure S4| The normalized PL excitation (PLE) spectra of CTFQD-160 with varying detection emission wavelengths (λ_{de}).

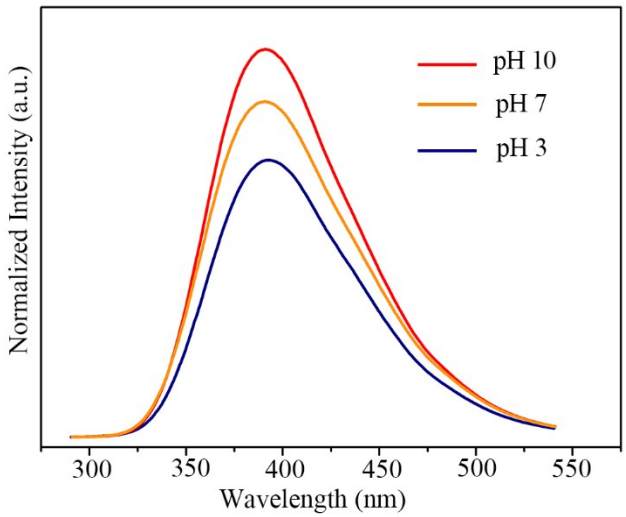

Figure S5| The PL spectra of CTFQD-160 at different pH. (excited at 290 nm).

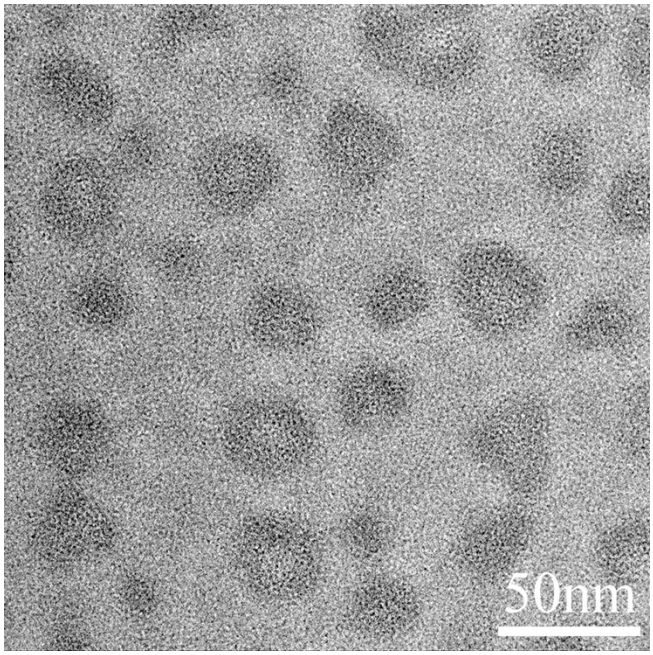

Figure S6| The TEM image of CTFQD-160 after hydrothermal treatment.

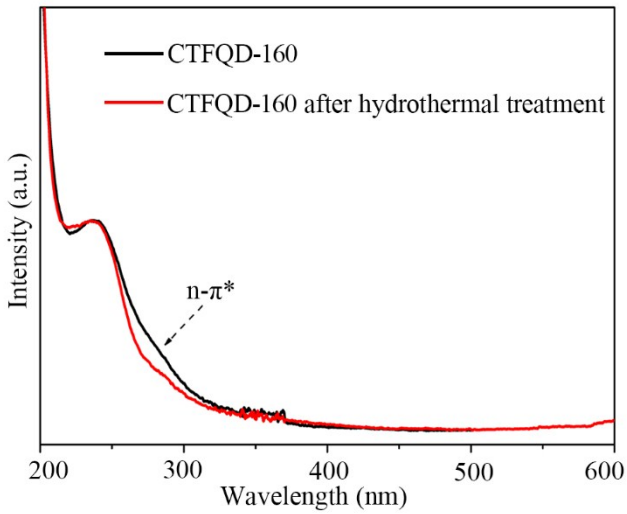

Figure S7| The UV-Vis spectra of CTFQD-160 before and after hydrothermal treatment.

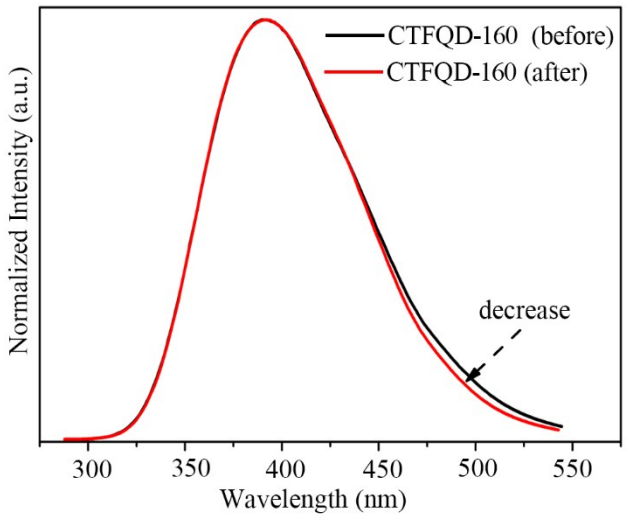

Figure S8| The normalized PL spectra of CTFQD-160 before and after hydrothermal treatment (excited at 290 nm).

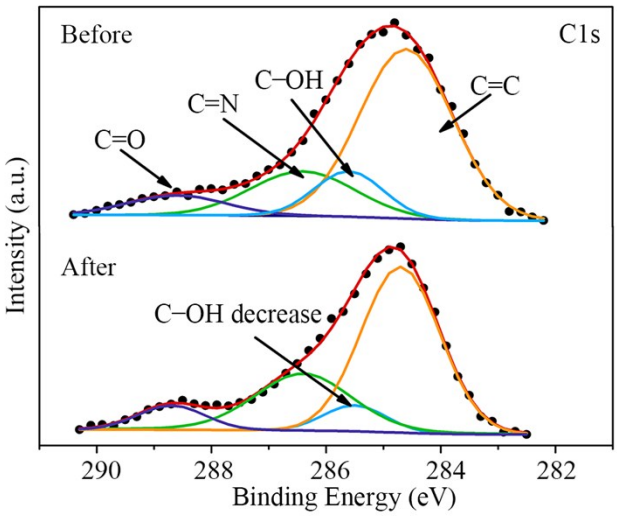

Figure S9| The C1s X-ray photoelectron spectroscopy (XPS) of CTFQD-160 before and after hydrothermal treatment.

Reference

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