Supporting Information

Light-Emitting Ti_2N (MXene) Quantum Dots: Synthesis, Characterization and Theoretical Calculations

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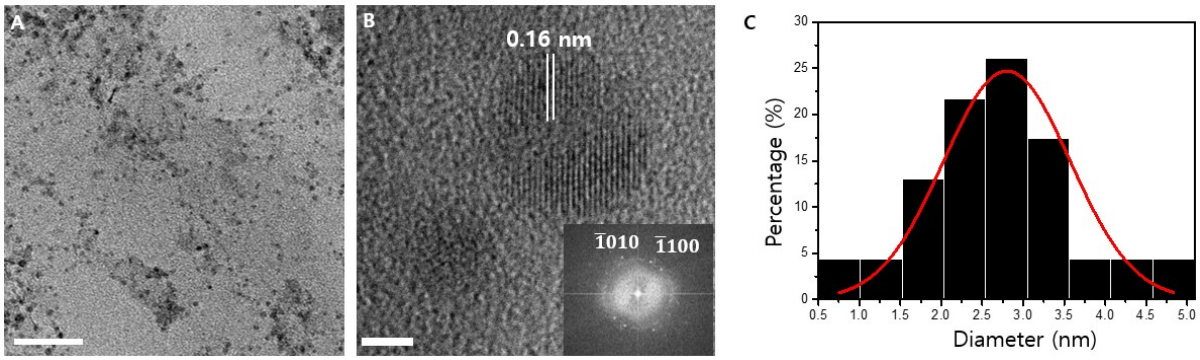

Figure S1: A. TEM image (scale bar = 50 nm) of Ti_2C MQDs. B. HR-TEM image (scale bar = 2 nm) of Ti_2C MQDs C. Size distribution of Ti_2C MQDs in (A). Inset of (B) is the FFT pattern of the corresponding HR-TEM image

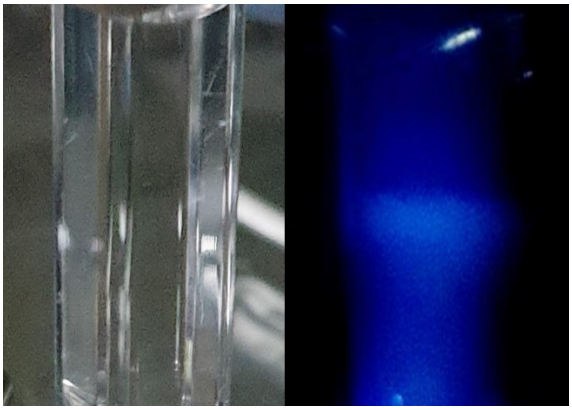

Figure S2: Fluorescence of Ti_2N MQDs dispersed in water. The MQDs showed blue emission when illuminated with UV (250 nm) LEDs.

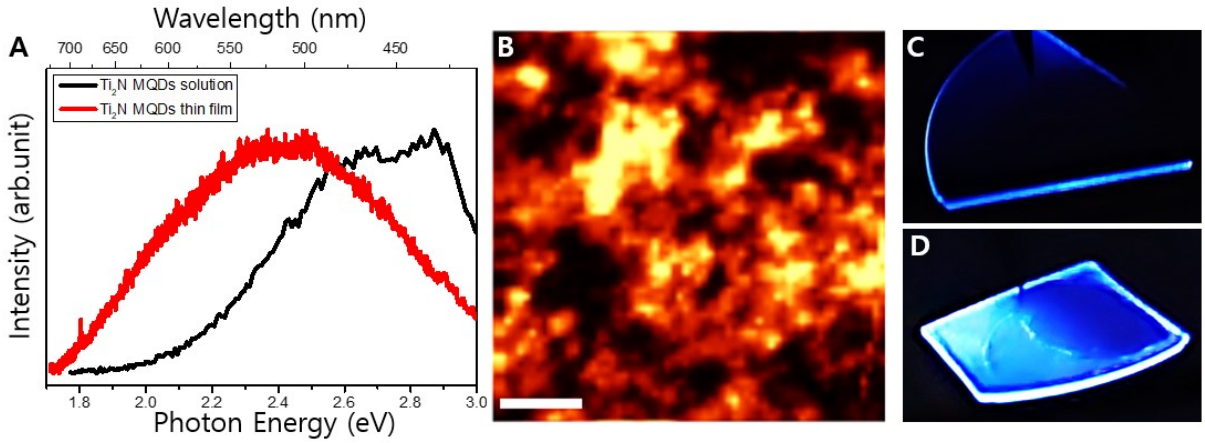

Figure S3: A. PL-spectrum of Ti_2N MQDs solution (black) and thin film (red) at 375-nm laser excitation B. Confocal image (scale bar = 5 µm) of thin-film Ti_2N MQDs at 405-nm laser excitation. C. Blank quartz substrate illuminated with UV (250 nm) LED D. Thin-film Ti_2N MQDs drop casted on quartz substrate illuminated with UV (250 nm) LED.

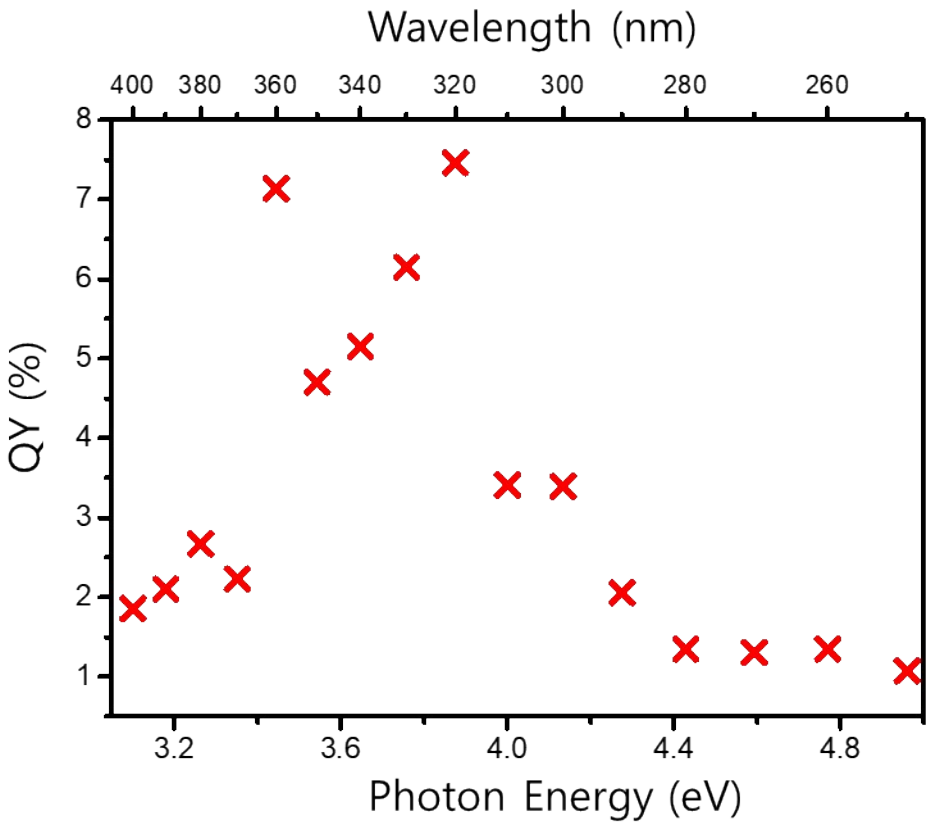

Figure S4: Plot of Ti_2N MQDs QY estimation vs. excitation energy (ranging from 250–400 nm wavelength excitation)

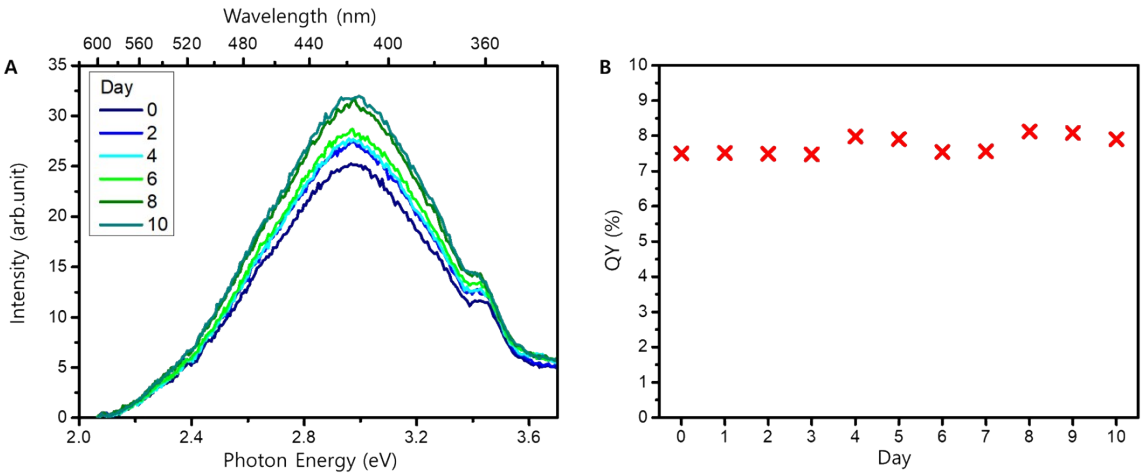

Figure S5: (A) PL intensity and (B) QY of Ti_2N MQDs in 10 days.

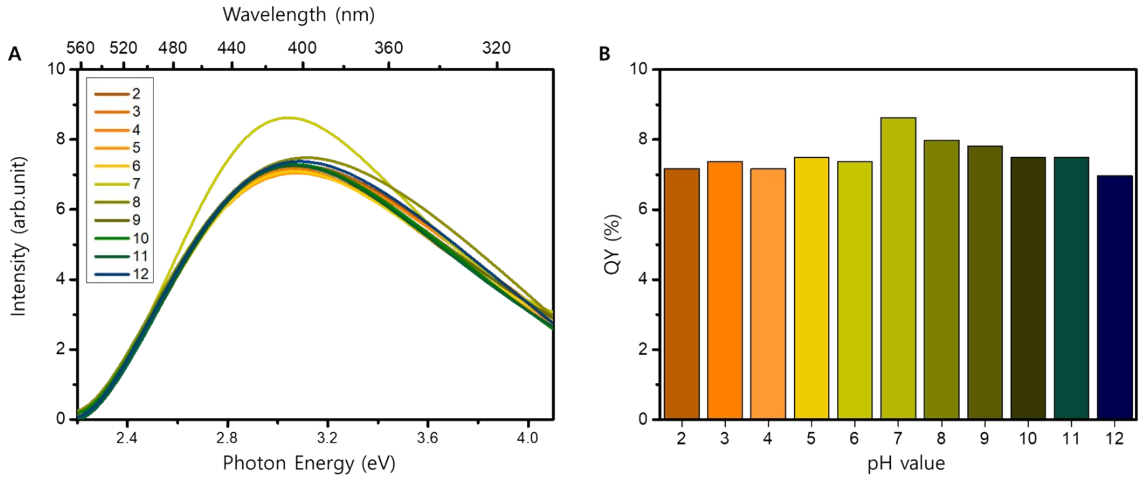

Figure S6: (A) PL spectra and (B) QY of Ti_2N MQDs in different pH condition ranging 2 – 12.

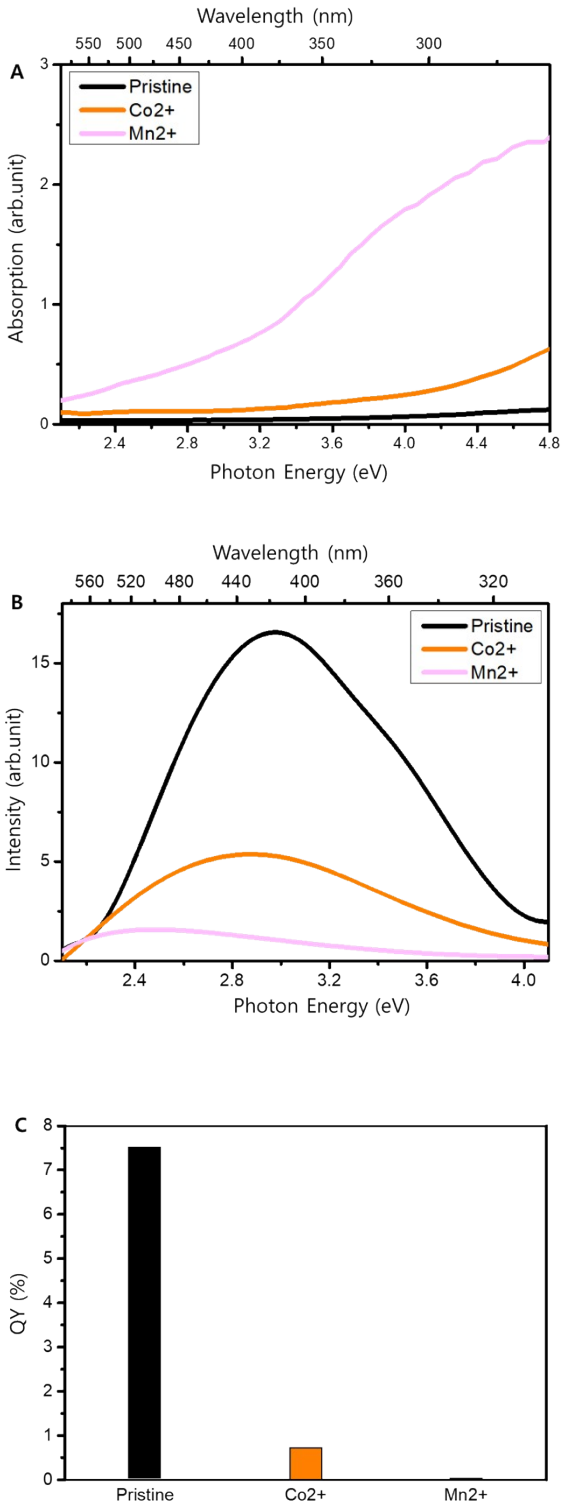

Figure S7: (A) UV-Vis absorption spectra, (B) PL spectra and (C) QY of Ti_2N MQDs with the presence of Co^{2+} and Mn^{2+} ions.

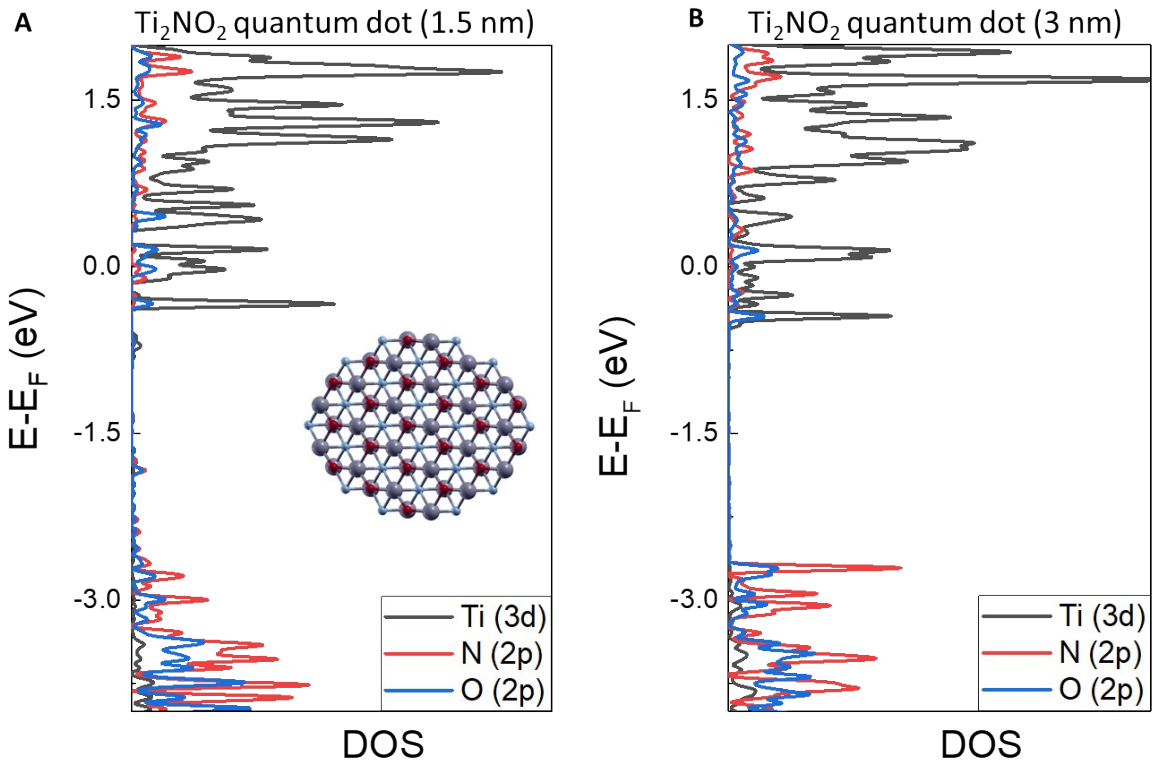

Figure S8: DFT calculation of Ti_2NO_2 MQDs with sizes of (A) 1.5 nm and (B) 3 nm.

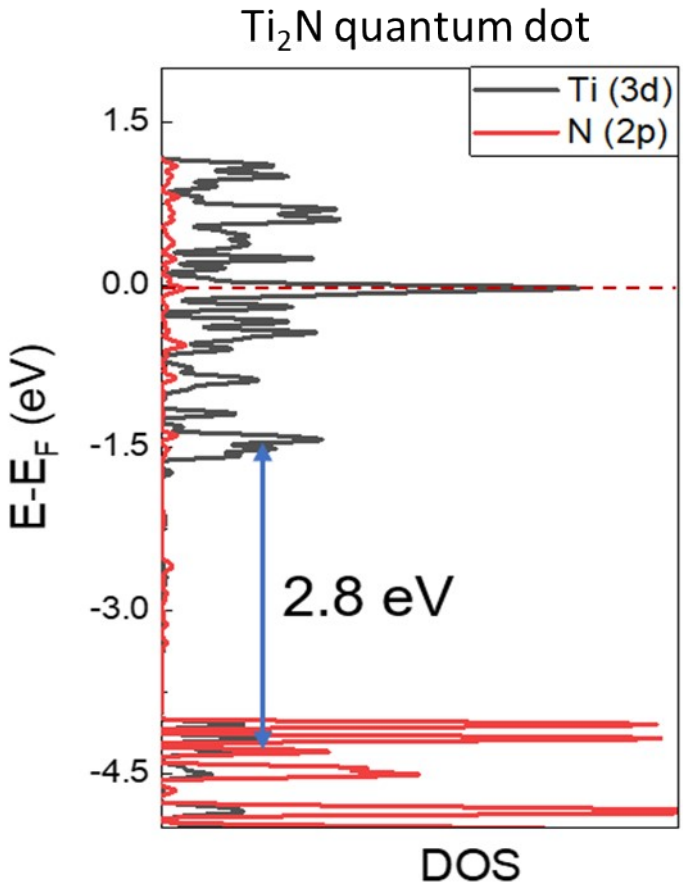

Figure S9: DFT calculation of Ti_2N MQDs.

Supporting note Figure S3:

We further confirmed the light-emitting property and PL behavior of thin-film Ti_2N MQDs for comparison with the PL of the Ti_2N MQD solution using a 375 nm laser (Figure S3A). The PL showed a redshift of the peak position when the colloidal solution was changed to a solid-state.[1] The PL confocal mapping of the thin film (Figure S3B) was performed using 405 nm laser excitation. The longer wavelength allowed proper observation of the PL of Ti_2N in solution. By illuminating the blank quartz substrate and thin-film Ti_2N MQDs using a UV (250 nm) LED, we demonstrated the light-emissive properties of the MQDs (Figures S3C and S3D).

Supporting note Figure S4: Measurement of Quantum Yield

We measured the absolute quantum yield (QY) of rhodamine 6G (R6G) solution in an integrating sphere and at different excitations using a commercial QY spectrometer. The PL and UV-Vis absorption of R6G and Ti_2N MQDs were measured under the same conditions, which were then compared to estimate the QY of the MQDs using Equation (1)[2] :

$$\Phi_{MQD} = \Phi_{ref} \frac{I_{(MQD)} / A_{(MQD)}}{I_{(ref)} / A_{(ref)}}$$

(1)

where ϕ_{MQD} and ϕ_{ref} are the QY of the MQDs and reference sample, respectively. $I_{(MQD)}$ is the PL intensity of the MQDs, $I_{(ref)}$ is the PL intensity of the reference sample, and $A_{(MQD)}$ and $A_{(ref)}$ are the absorptions of the MQDs and reference sample, respectively. The QY (%) of Ti_2N were calculated within the range of 250 to 400 nm wavelength excitation. For this measurement, the R6G solution was used as the reference sample.

References

1 T. E. Saraswati, U. H. Setiawan, M. R. Ihsan, I. Isnaeni and Y. Herbani, *Open Chem.*, 2019, **17**, 1198–1212.

2 S. Roy, A. S. Sharbirin, Y. Lee, W. Bin Kim, T. S. Kim, K. Cho, K. Kang, H. S. Jung and J. Kim, *Nanomaterials*, 2020, **10**, 1032.