Tuning colloidal tungsten dichalcogenide nanomonolayers bandgap by controlling their size and composition

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Group 6 transition metal dichalcogenides are a promising family of materials with a tunable bandgap, a stable and a metastable phase, and a large surface area in the form of monolayers, which makes them an exceptional choice for different applications such as electronics, optoelectronics, and electrocatalysts. Bandgap tailoring is achievable by reducing the size of the material to monolayer thickness or by alloying[1]. Engineering the crystal structure of transition metal dichalcogenides is crucial for controlling the electronic and optoelectronic properties of these materials. Here, we report a colloidal protocol to produce size-controlled and well-dispersed nanomonolayers (NMLs) of 1T'-WS_2 and 1T'-WSSe in the size range 10-70 nm, and we investigate the phase transformation into the 2H structure on the different sizes. TEM and STEM images demonstrate the well-dispersed monodisperse nanomonolayers of 1T'-WS_2 and 1T'-WSSe (changing the reaction parameters causes a change in the mean size). Figure 1a and c show the low magnification STEM images of well-dispersed 1T'-WS_2 NMLs, and b and d demonstrate high magnification ones. X-ray photoemission spectroscopy and X-ray diffraction confirm the phase transformation from 1T' to 2H. UV-vis spectroscopy supports the phase change and exhibits the bandgap change either by alloying or by controlling the mean size (Figure 1e and f). Hypsochromic shift happens by reducing the size of nanosheets due to quantum confinement. In conclusion, we developed a new colloidal protocol to produce size-controlled and well-dispersed NMLs of semi-metallic WS_2 and WSSe, then change the structure to semiconducting and investigate the bandgap change due to the change in diameters and composition.

References

[1] Shahmanesh, Ashkan, et al. "2D Monolayer of the 1T'Phase of Alloyed WSSe from Colloidal Synthesis." *The Journal of Physical Chemistry C* 125.20 (2021): 11058-11065.
[2] Sokolikova, Maria S., and Cecilia Mattevi. "Direct synthesis of metastable phases of 2D transition metal dichalcogenides." Chemical Society Reviews 49.12 (2020): 3952-3980.

Figures

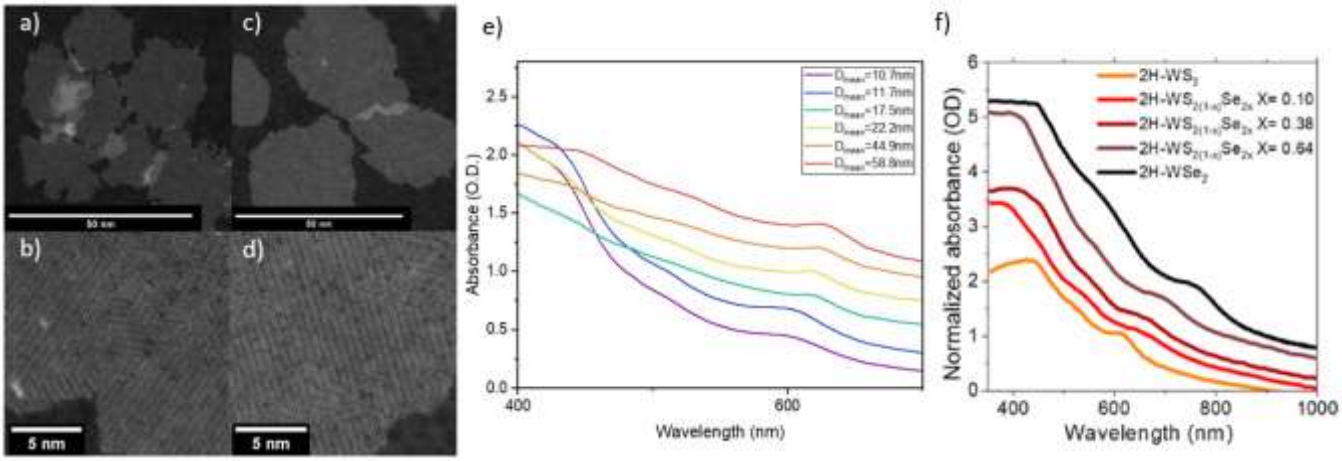

Figure 1: HAADF-STEM image of monolayers of 1T'-WS_2 with different mean sizes: a,b) 22.2 nm, c,d) 58.8nm. e) Absorption spectra of different sizes 2H-WS_2. F) Absorption spectra of 1T'-WSSe with different selenium content.