

Supporting Information

Hybrid chalcogenide nanoparticles: 2D-WS₂ nanocrystals inside nested WS₂ fullerenes

Faegheh Hoshyargar,^a Tomas P. Corrales,^c Robert Branscheid,^b Ute Kolb,^b Michael Kappl,^c

*Martin Panthöfer,^a Wolfgang Tremel^{*a}*

^a Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universität, Duesbergweg 10-14, D-55128 Mainz, Germany. Fax: +49 6131 / 39-25605; Tel: +49 6131 / 39-25135; E-mail: tremel@uni-mainz.de

^b Institute für Physikalische Chemie, Johannes Gutenberg-Universität, Welderweg 11, D-55128 Mainz, Germany.

^c Max Planck Institute für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany.

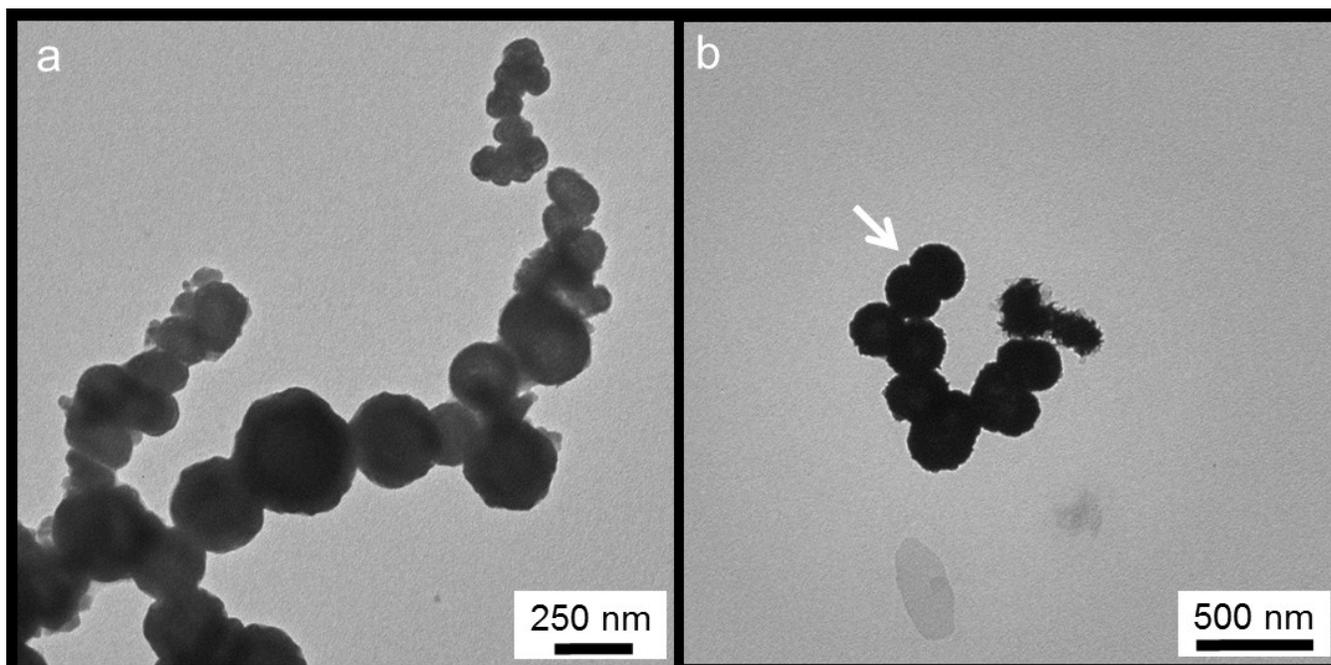


Figure S1. TEM images of the primary product obtained after the first step at 600°C. (a) Clusters of spherical particles, (b) Intergrown spherical particles (shown by an arrow).

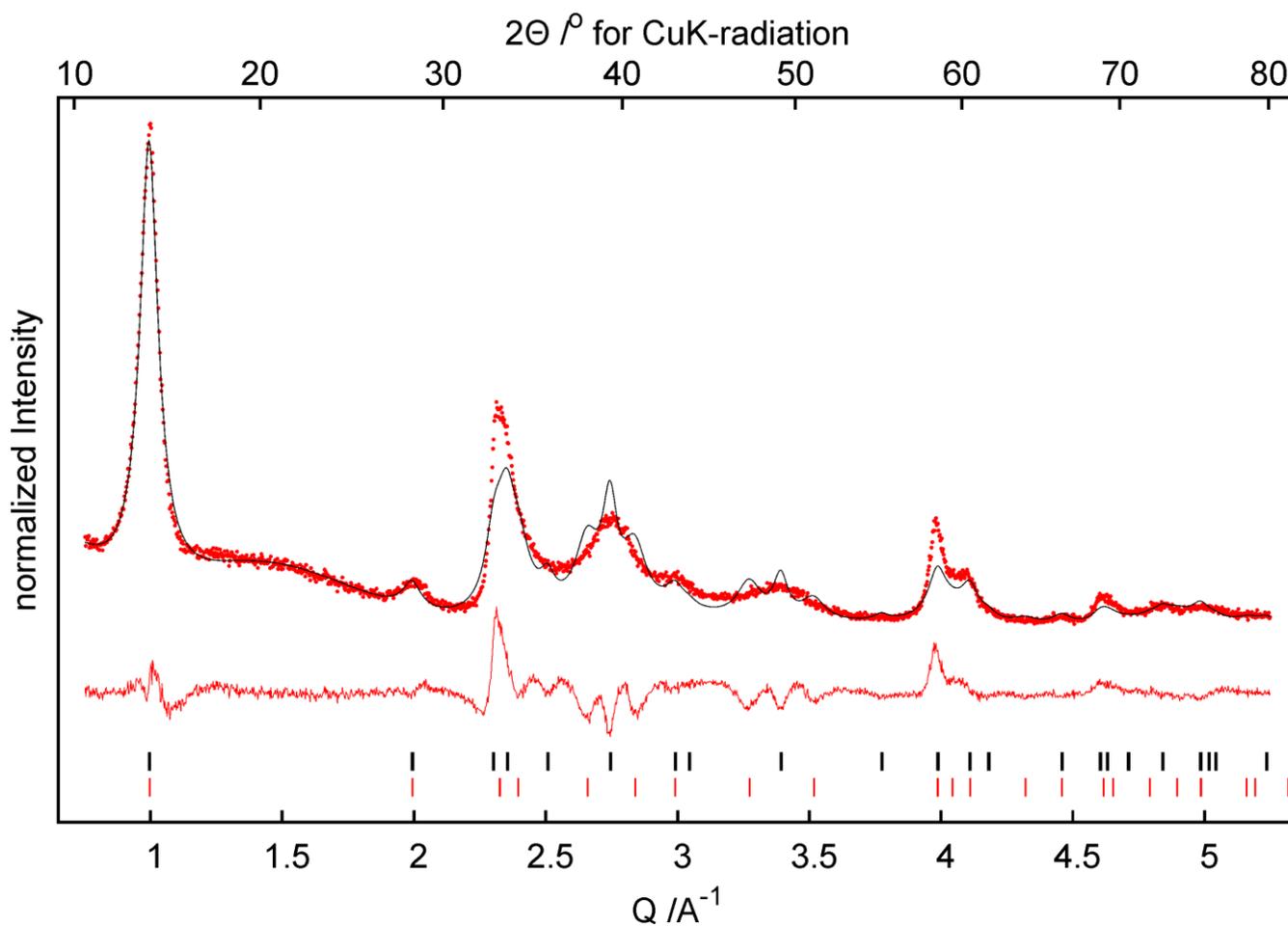


Figure S2. Rietveld-refinement of the x-ray diffraction pattern of the final product (red dots: observed intensity, black line: model, red line: difference curve, ticks marks the reflection positions of $2H\text{-WS}_2$ (black, W.J. Schutte, J.L. DeBoer, F. Jellinek, *J. Solid State Chem.* 1987, **70**, 207-209) and $3R\text{-WS}_2$, (F. Jellinek, J.C. Wildervanck, *Z. Anorg. Allg. Chem.* 1964, **328**, 309-318).

Table S1. Measurement and refinement parameter of the Rietveld refinement of the final product

Diffractometer	Siemens D5000
Sample preparation	Fine powder fixed between two stripes of Scotch™ tape
Measuring mode	Transmission
Wavelength	1.540596
Measuring range	$10 \leq 2\Theta /^\circ \leq 90$; $0.71 \leq Q / \text{\AA}^{-1} \leq 5.77$
Temperature /K	298K
Profile Fit	Rietveld refinement according to reported crystal structure models
Background / Parameters	Chebyshev / 15
Profile function	Fundamental Parameters Approach
Program	TOPAS Academic V5.1
Total No. of Parameters	23
R_{exp}	4.6
R_{wp}	13.0
GoF	2.86
Phase I	WS ₂ -2H
Space group	<i>P6₃/mmc</i>
Cell parameters / Å	a = 3.151(1) Å, c = 12.600(5) Å
Crystallite size / nm	10(1)
Fraction /%wt	34(2)
Biso	2.8(1)
Phase II	WS ₂ -3R
Space group	<i>R3m</i> (hexagonal setting)
Cell parameters / Å	a = 3.151(1) Å, c = 18.900(5) Å
Crystallite size / nm	6(1)
Fraction /%wt	66(2)
Biso	2.8(1)

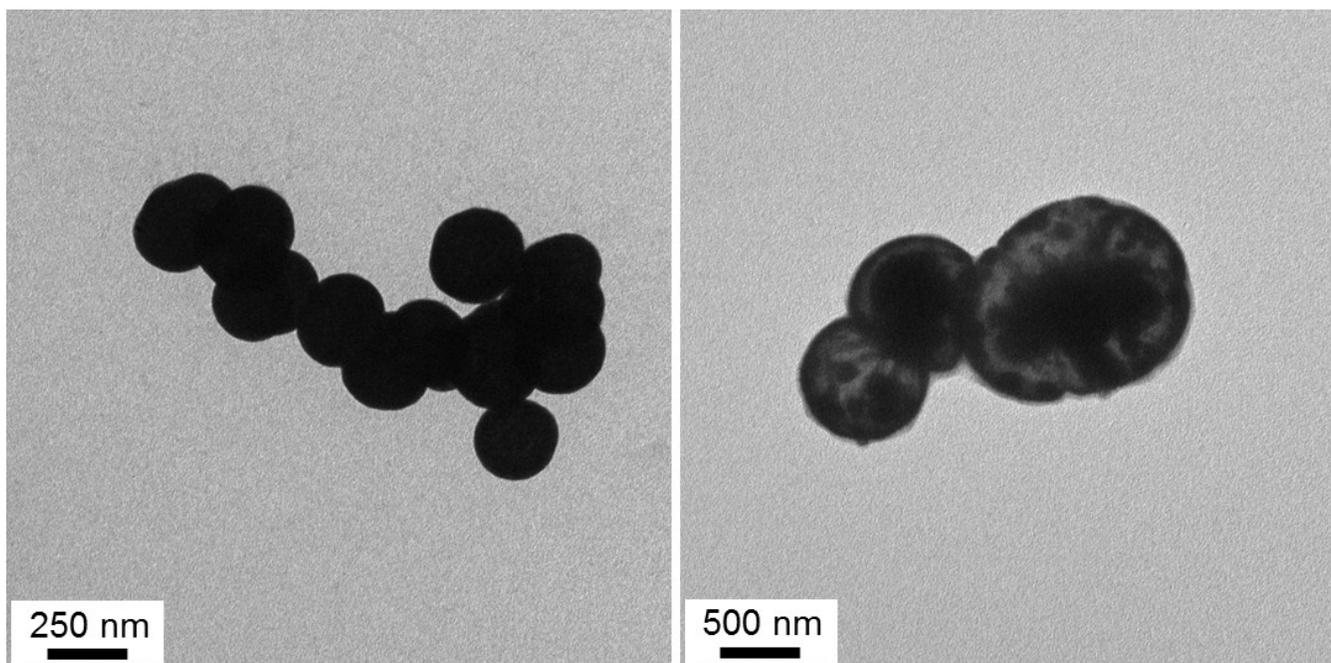


Figure S3. TEM overview image of the product obtained at the annealing temperature of 750°C

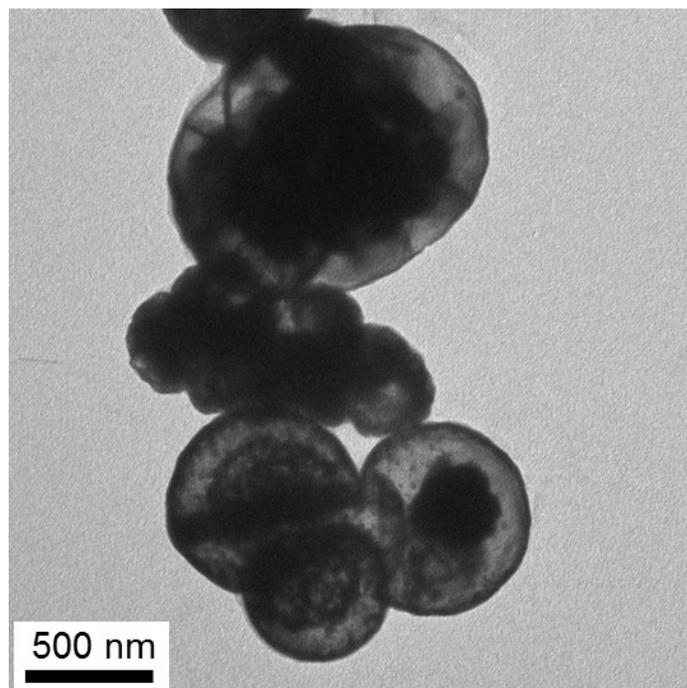


Figure S4. TEM overview image of the product obtained at the annealing temperature of 800°C.

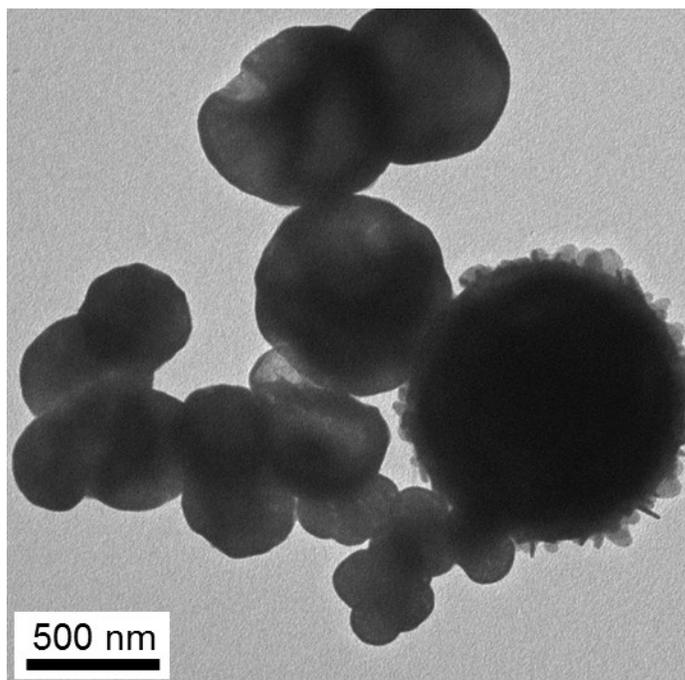


Figure S5. TEM overview image of the product obtained at the annealing temperature of 900°C.

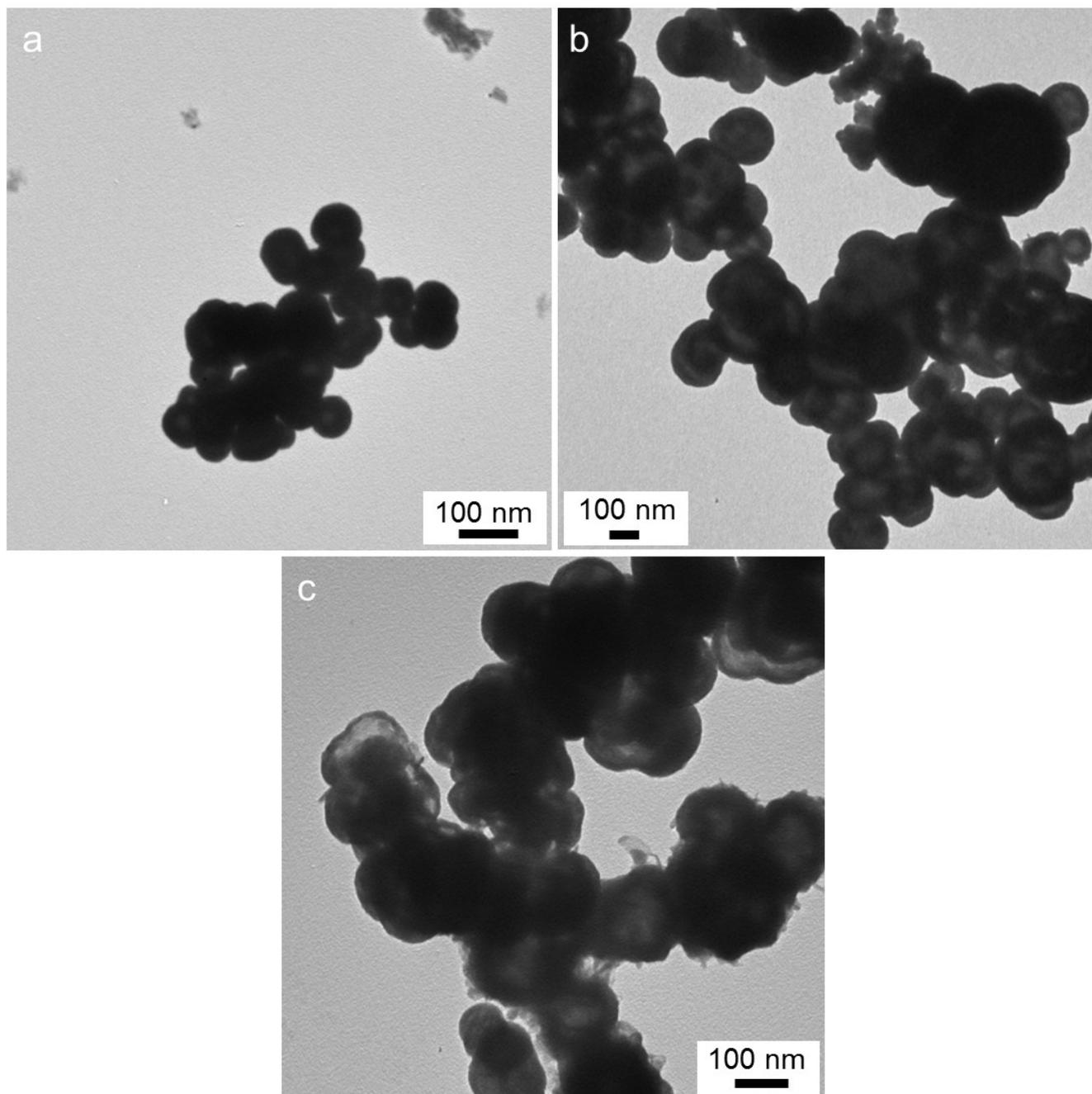


Figure S6. TEM images of the products obtained from reactions at (a) 300°C, (b) 400°C and (c) 500°C.

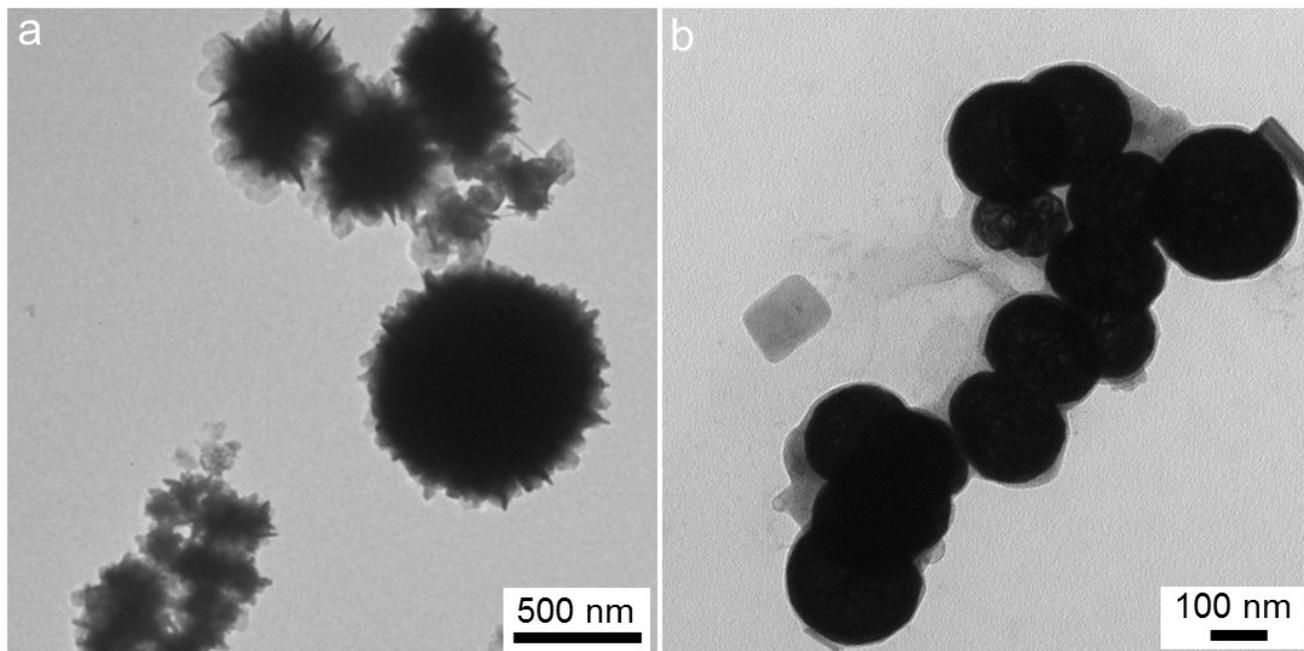


Figure S7. TEM image of the annealed product obtained (a) without iodine and (b) for a $W(CO)_6/I_2$ ratio of 1:1.

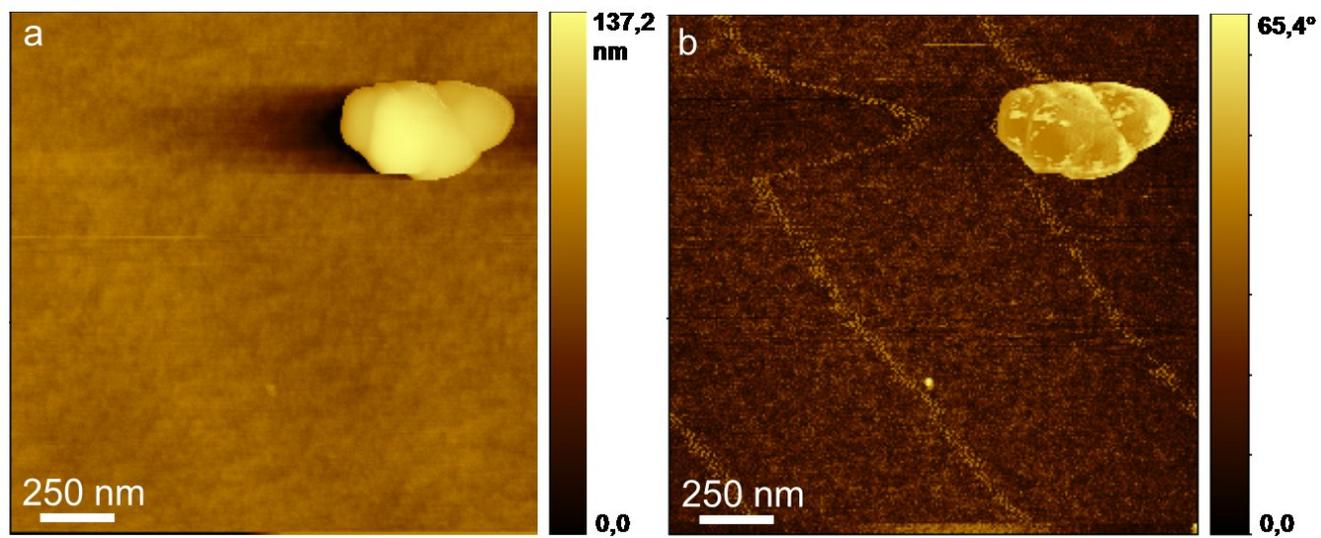


Figure S8. (a) AFM height profile of as-synthesized IF-WS₂ particle. (b) Phase profile of IF-WS₂ particles.