

## Redox exfoliated NbS<sub>2</sub>: characterization, stability, and oxidation

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### Supporting Information (SI)

**Text S1.** The equations used to fit the absorbance spectra that generate the kinetics profile are described above.

#### Equations

Equation S1

$$A_t = (A_f - A_0) \times (1 - e^{-k_1 t}) + A_0$$

Where:

$A_f$  = final absorbance of oxidation process

$A_0$  = initial absorbance of oxidation process

$k_1$  = formation constant of NbSO

Equation S2

$$A_t = A \times \left( 1 - e^{-k_2 t} \right) + 1 + e^{\frac{\kappa_1}{(-\ln 81 \left( \frac{t - t_{m1}}{\Delta t_1} \right))}} + 1 + e^{\frac{\kappa_2}{(-\ln 81 \left( \frac{t - t_{m2}}{\Delta t_2} \right))}}$$

Where:

$A$  = absorbance constant

$k_2$  = formation constant of NbSO

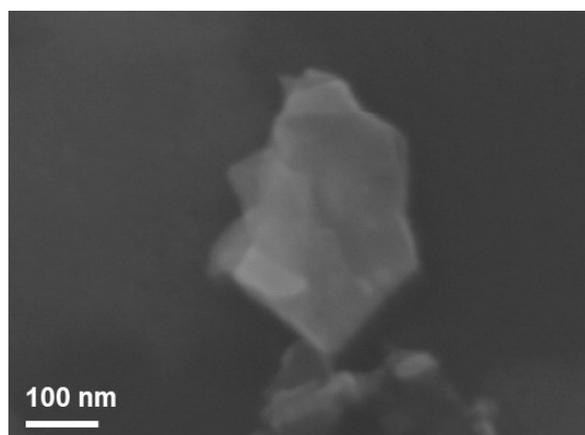
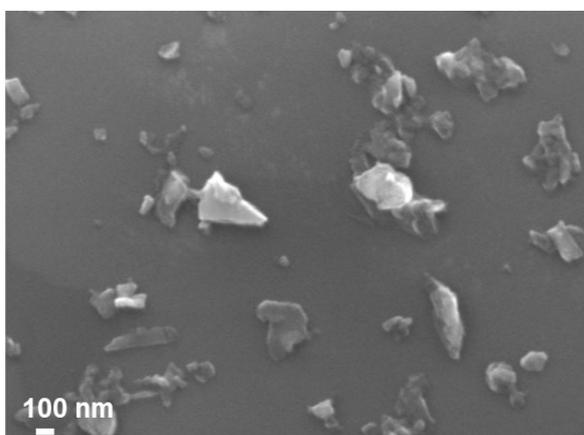
$\kappa_1$  and  $\kappa_2$  = asymptotic absorbance values

$\Delta t_{1,2}$  = midpoint time of the respective processes

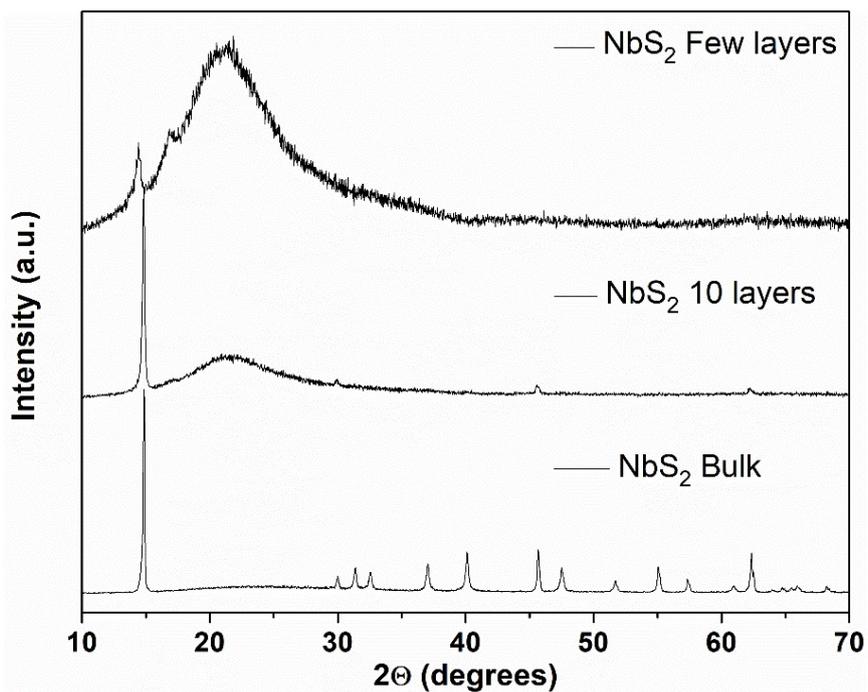
$t_{m1,2}$  = characteristic formation times

Table S1. Kinetic parameters obtained by fitting data in Figure 7c according to Biologistic Model, Equation S2.

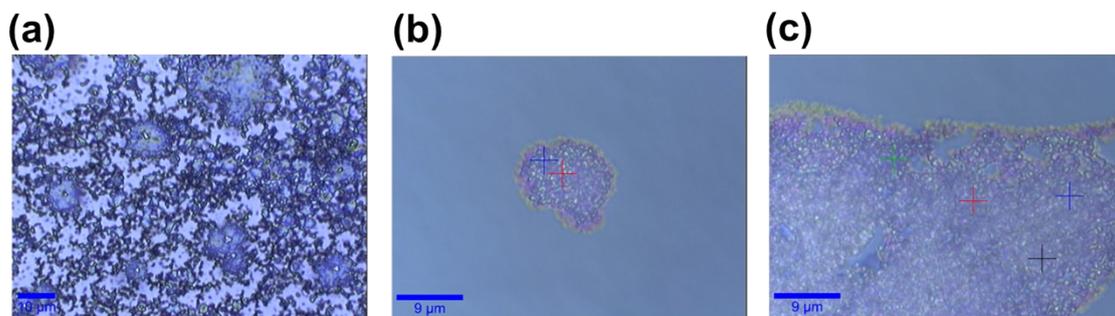
Kinetic parameter	Values
$\kappa_1$	$0.62806 \pm 0.03528$
$\Delta t_1$	185.9 s
$t_{m1}$	375.83 s
$\kappa_2$	$0.13664 \pm 0.02311$
$\Delta t_2$	15.5 s
$t_{m2}$	235.3 s
$k_2$	$2.5 \times 10^{-4} \text{ s}^{-1}$



**Figure S1.** Scanning electron microscopy (SEM) of the FL-NbS<sub>2</sub> obtained.



**Figure S2.** X-Ray diffraction (XRD) comparison between NbS<sub>2</sub> bulk and FL-exfoliated.



**Figure S3.** Optical images of the NbS<sub>2</sub>: (a) exposed sample before annealing, (b) and (c) different clusters formed after annealing, small and larger respectively.

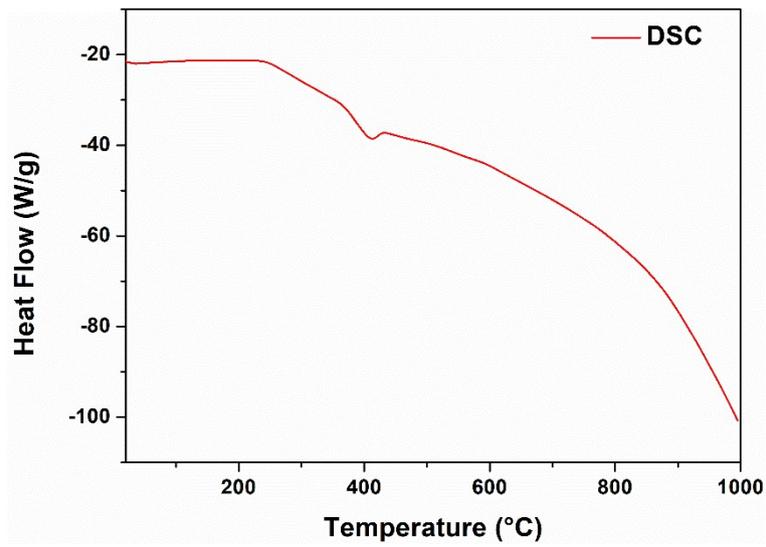


Figure S4. Differential scanning calorimetry (DSC) of the FL-NbS<sub>2</sub>.

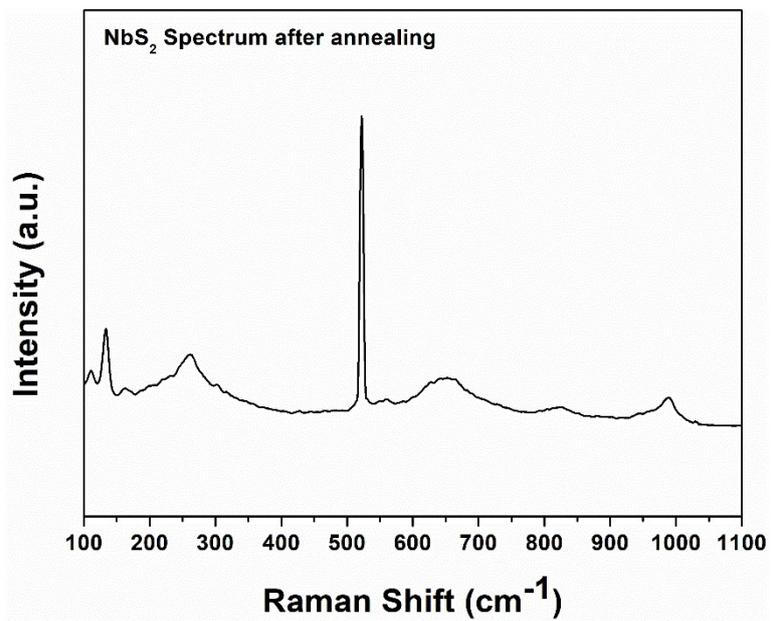


Figure S5. Raman modes after thermal annealing of the sample (NbS<sub>2</sub>).

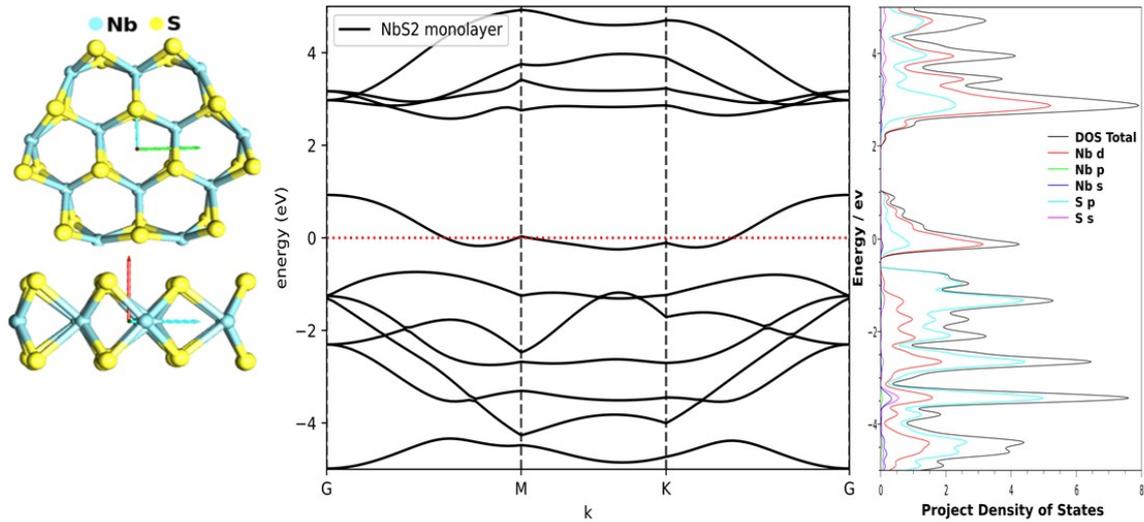


Figure S6. Projected band structure for the NbS<sub>2</sub>.

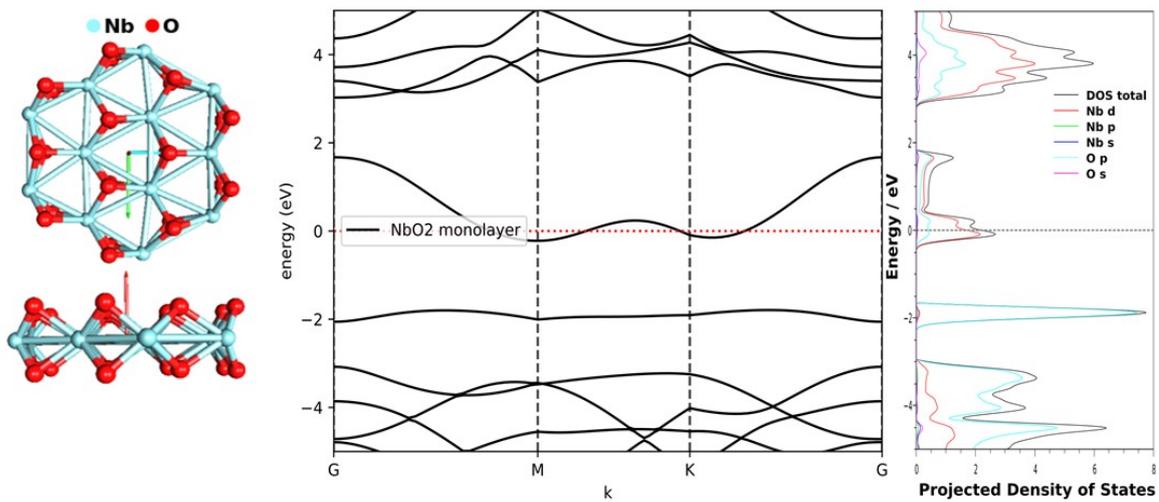
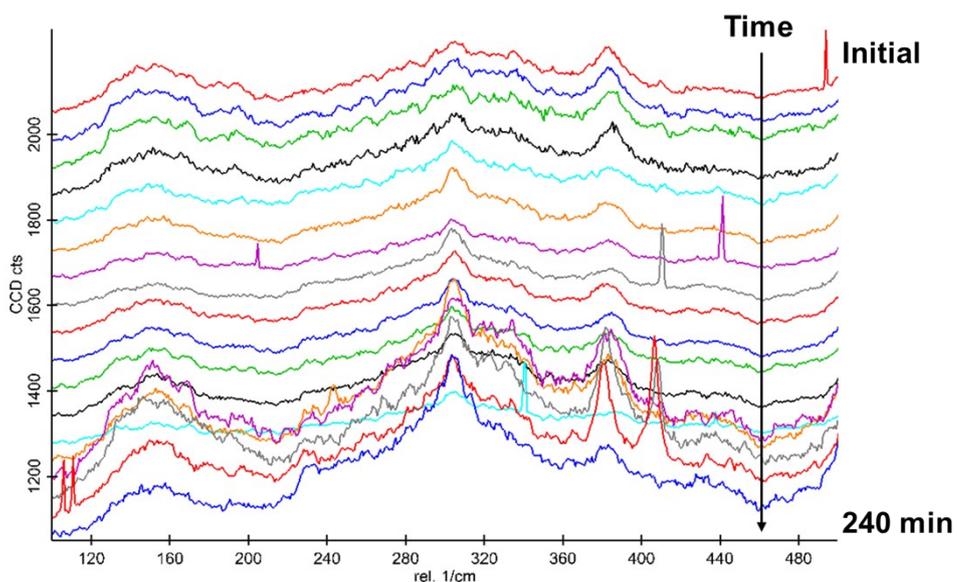


Figure S7. Projected band structure for the NbO<sub>2</sub>.



**Figure S8.** Raw Raman spectra of the redox exfoliated NbS<sub>2</sub> for various exposure times to ambient conditions. Time evolves from top to bottom, where the top spectrum corresponds to the sample measured in an inert environment and the last corresponds to the spectrum after 240 minutes of exposure.