Supplementary Materials for

Batch growth of wafer scale nanocrystalline $NbSe_2$ film for surface-enhanced Raman spectroscopy

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This Supplementary Information includes the following sections:

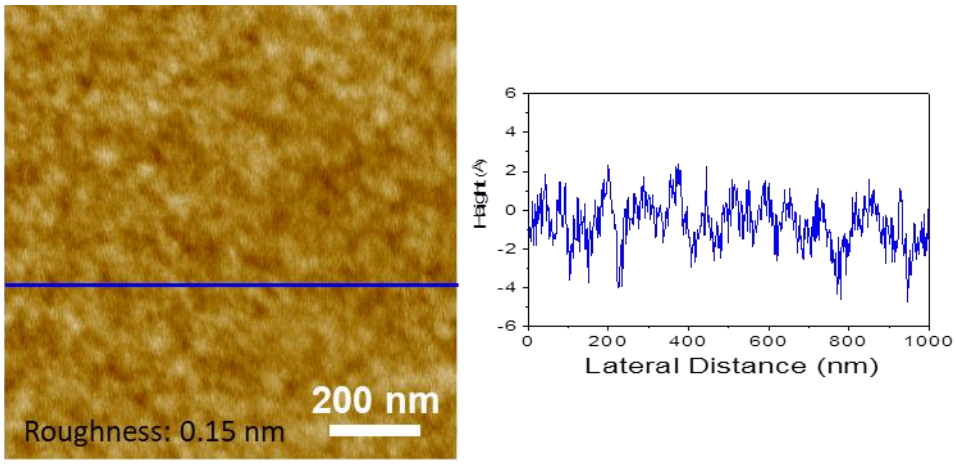

Figure S1. The roughness of Nb film sputtered on SiO_2/Si. AFM image (Left) and the corresponding height profile of a nanocrystalline Nb film sputtered on SiO_2/Si (Right) at room temperature.

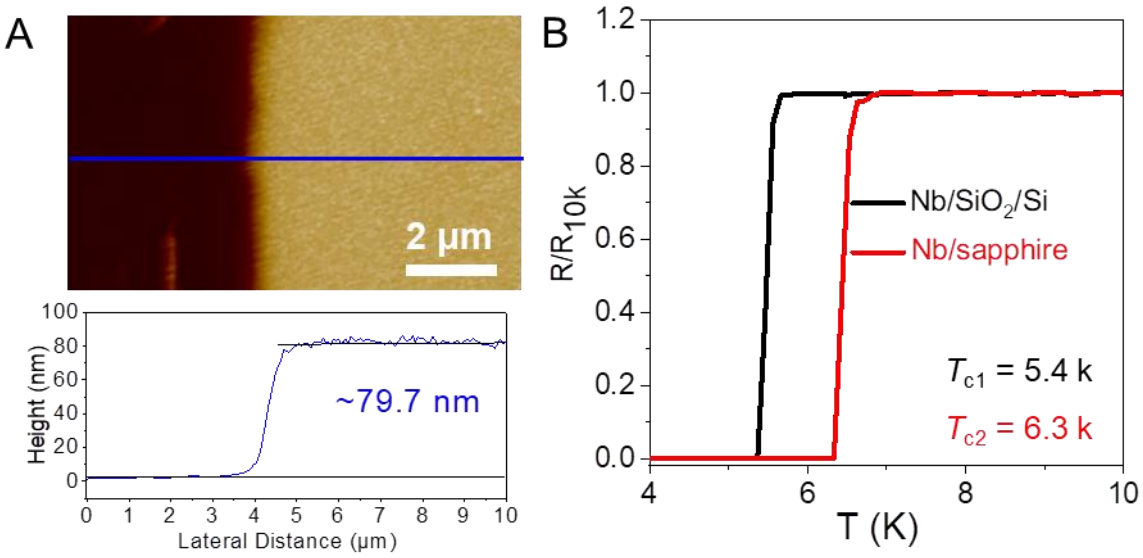

Figure S2. Substrate-dependent crystalline quality of as-sputtered Nb films at the same sputtering conditions. (A) AFM image and the corresponding height profile of an as-sputtered Nb film. (B) Superconductivity of the Nb films on SiO_2/Si and sapphire under the same sputtering conditions (e.g., sputtered at room temperature). Note: The superconducting transition critical temperature (T_c): the temperature at which the sheet resistance drops to 10% of its normal state.

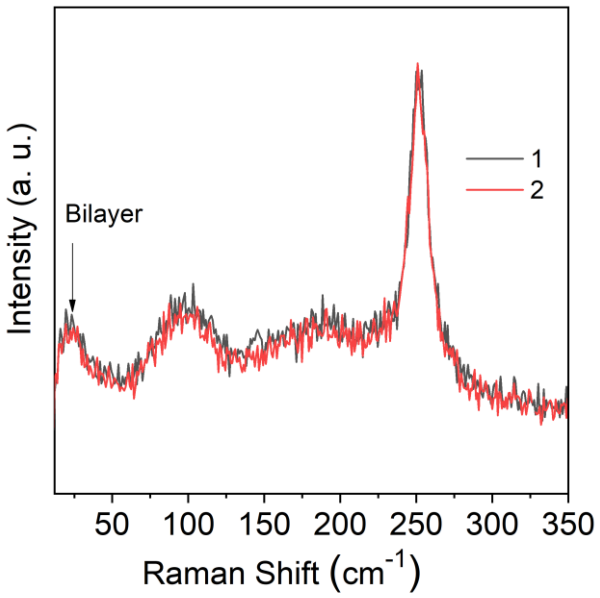

Figure S3. Raman spectra of NC-$NbSe_2$ film with perpendicular polarization.

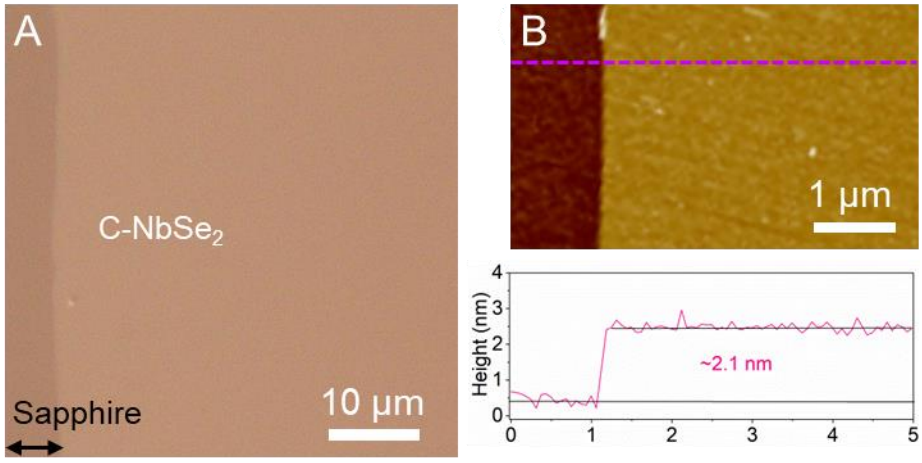

Figure S4. Morphology characterization of C-$NbSe_2$ films directly grown on sapphire. (A) optical microscopic image of as-grown C-$NbSe_2$ film on sapphire substrates. (B) AFM image and the corresponding height profile of C-$NbSe_2$ films directly grown on sapphire.

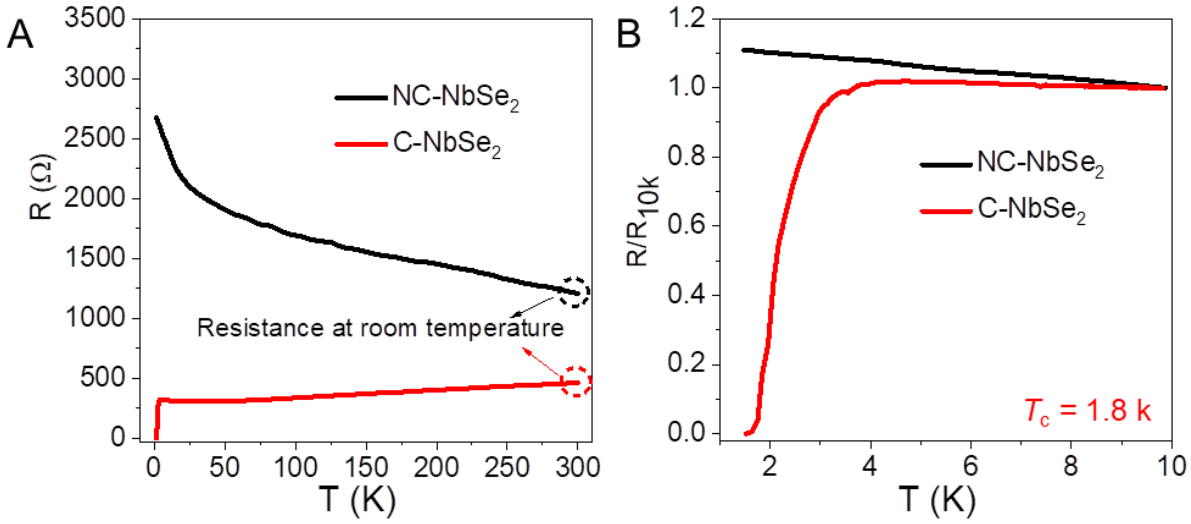

Figure S5. Substrate-dependent transport property of as-grown $NbSe_2$ films the same mild growth conditions. The temperature dependence resistance of $NbSe_2$ films on SiO_2/Si and sapphire (referred as NC-$NbSe_2$, NC-$NbSe_2$, respectively) at a mild growth temperature (550 ℃). The resistance of $NbSe_2$ films on SiO_2/Si and sapphire at room temperature are marked by a black dotted circle frame and a red dotted circle frame in (A), respectively. The resistance in (B) is normalized by the resistance at the temperature of 10 K (the normal state of Superconducting $NbSe_2$).

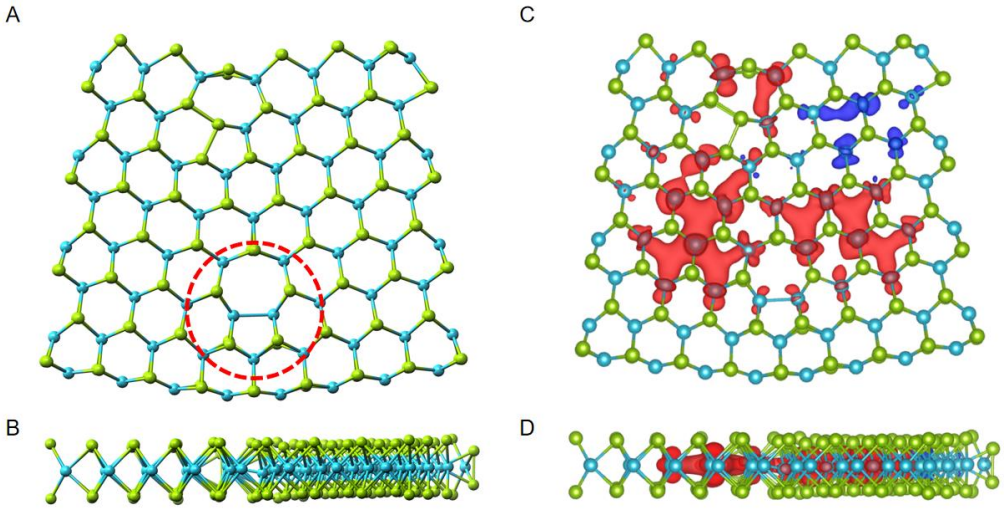

Figure S6. Atomic model structures of GBs of NC-$NbSe_2$. (A-B) Atomic model structures of GBs of NC-$NbSe_2$. (C-D) Spin density of GBs of NC-$NbSe_2$ (Spin up: red, spin down: blue, isosurface= ±0.002).

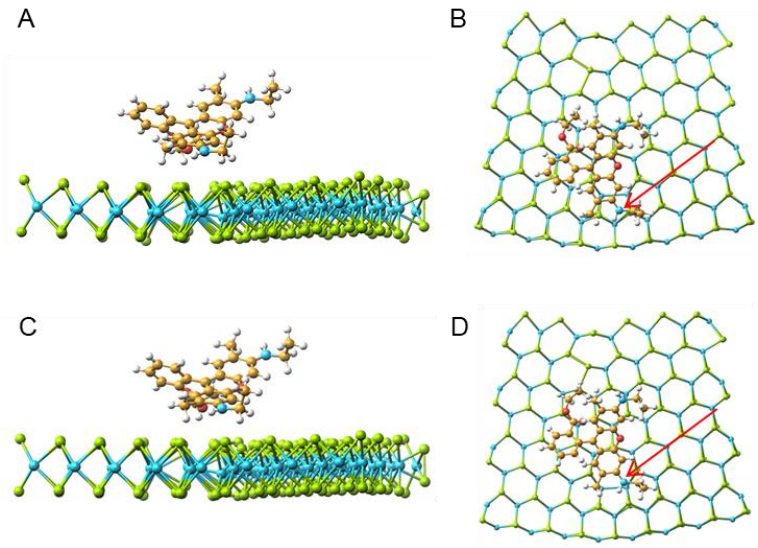

Figure S7. Origin of the SERS effect of NC-$NbSe_2$. Side-view and top-view of R6G molecules adsorbed on the NC-$NbSe_2$ surface, illustrating the adsorption configurations on (A, B) pentagonal rings, (C, D) heptagonal rings.

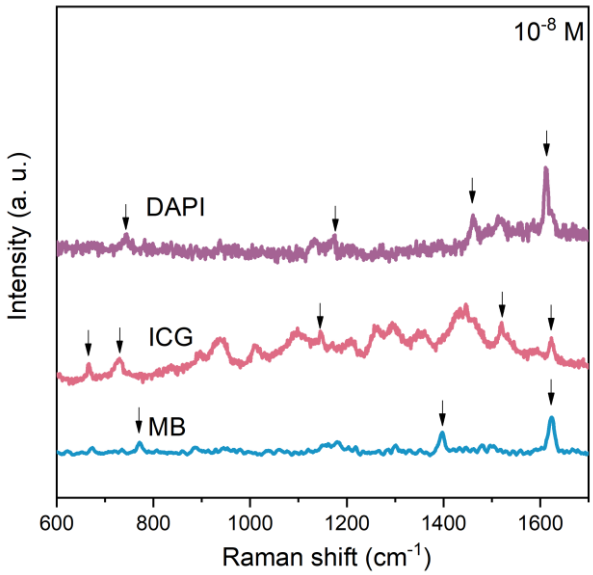

Figure S8. The SERS performance evaluation of NC-$NbSe_2$ film for different dyes. The Raman spectra for various dyes (1×10^{-8} M) on NC-$NbSe_2$ films, including indocyanine green (ICG), methylene blue (MB), 2-(4-Amidinophenyl)-6-indolecarbamidine dihydrochloride (DAPI).

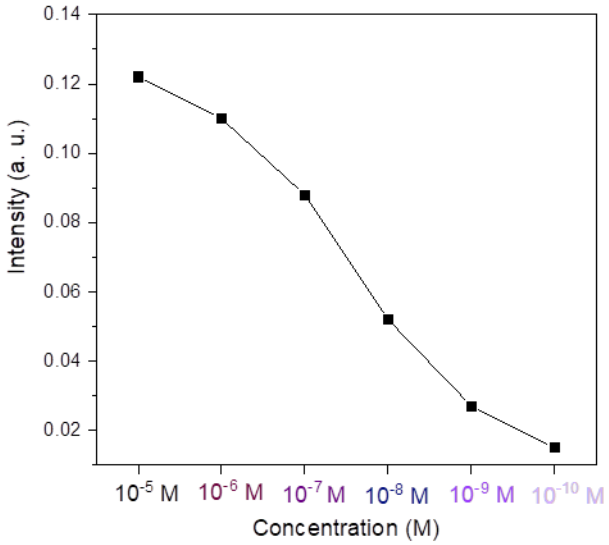

Figure S9. The SERS effect of as-grown NC-$NbSe_2$ film as a function of dye concentrations. Raman intensity at 1361 cm^{-1} as a function of R6G concentrations.

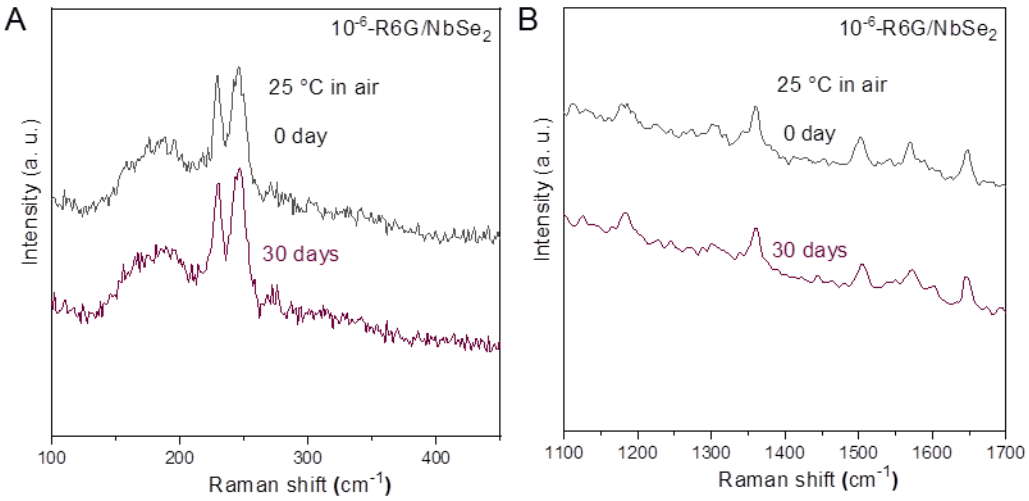

Figure S10. Air-stable SERS effect of as-grown NC-$NbSe_2$ film. The Raman spectra of (A) NC-$NbSe_2$ films and (B) coated R6G molecules before/after exposure to air for 30 days at 25 ℃.

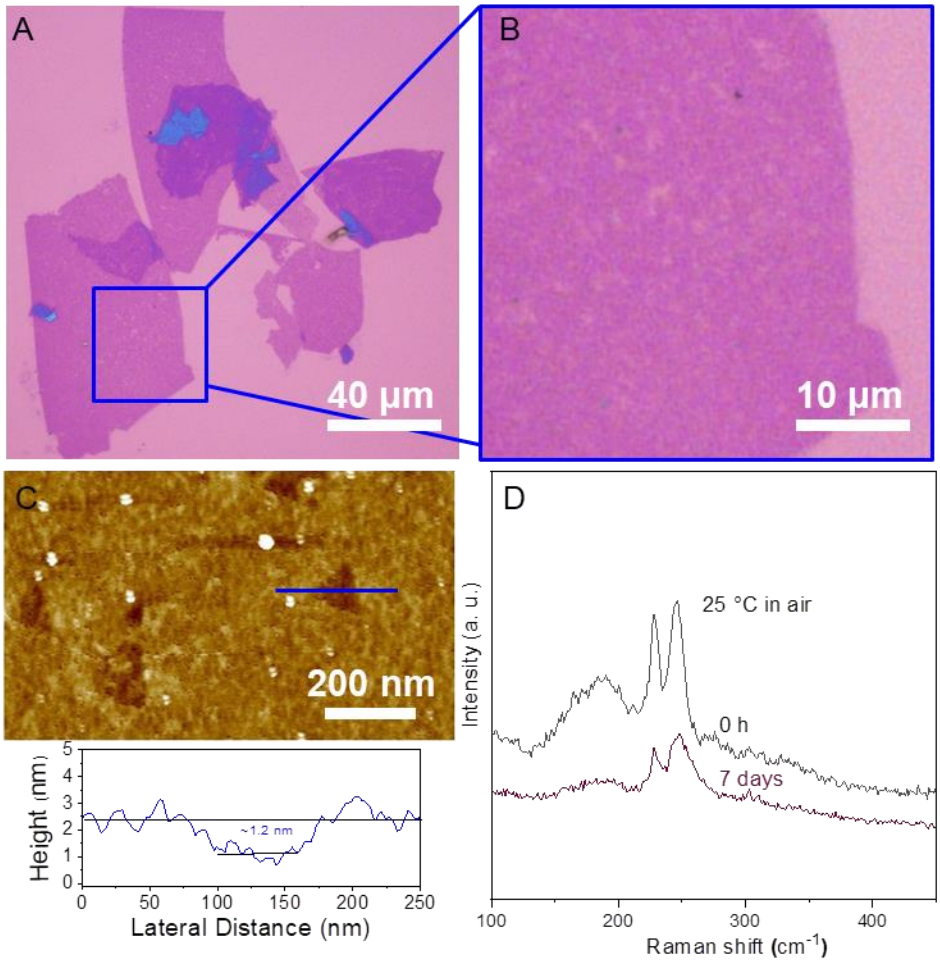

Figure S11. Instability of electrochemically exfoliated $NbSe_2$ flakes. (A, B) The optical images, (C) AFM image and the corresponding height profile, and (D) Raman spectra of electrochemically exfoliated $NbSe_2$ after exposure to air at 25 °C 7 days.

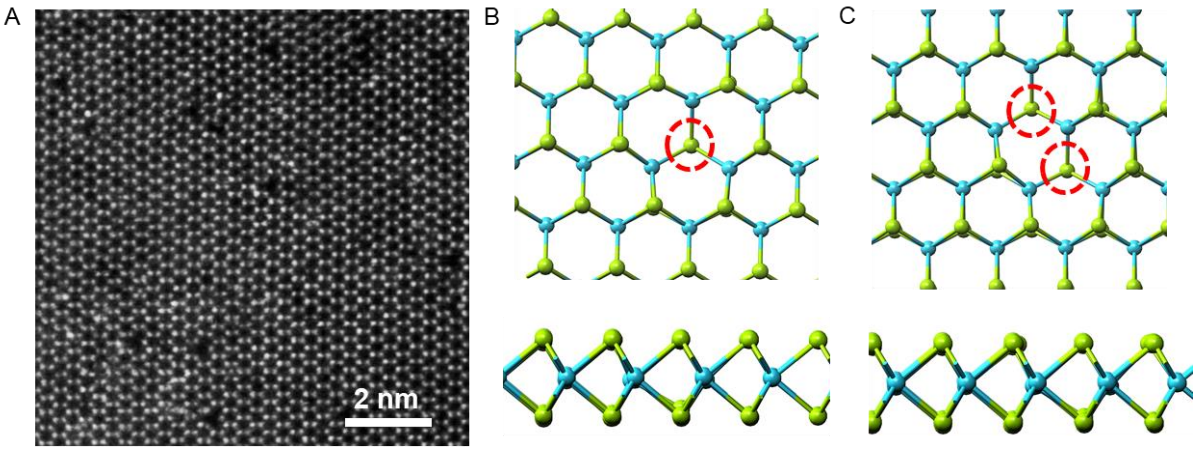

Figure S12. Origin of instability in electrochemically exfoliated $NbSe_2$ flakes. (A) ADF-STEM images of monolayer $NbSe_2$ after an exposure to air for few minutes. B, the sites of single Se vacancy and double Se vacancies created in monolayer $NbSe_2$ atomic model structures.

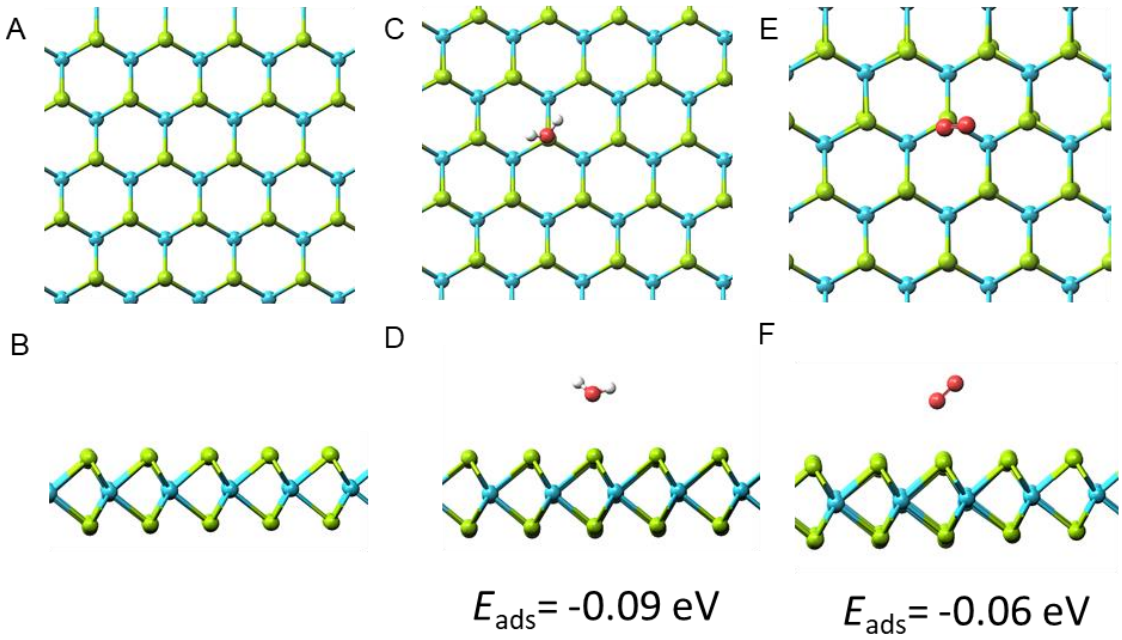

Figure S13. Pristine $NbSe_2$ flakes in air. Side-view and top-view of atomic model structures of (A, B) defect-free monolayer $NbSe_2$. (C, D) H_2O adsorbed on defect-free monolayer $NbSe_2$, (E, F) O_2 adsorbed on defect-free monolayer $NbSe_2$.

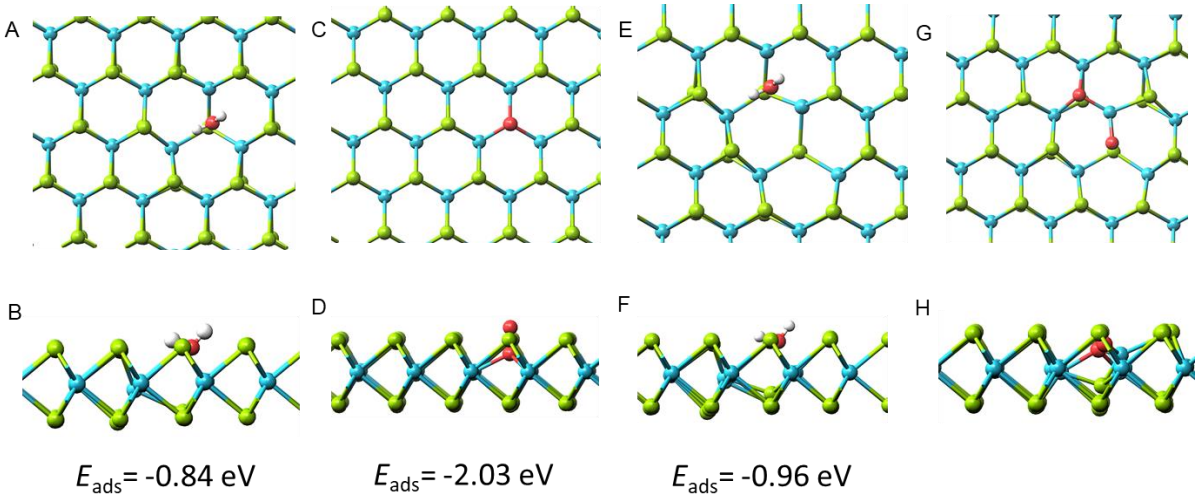

Figure S14. $NbSe_2$ flakes with points defect in air. Side-view and top-view of atomic model structures of H_2O (A, B) and O_2 (C,D) adsorbed on single Se vacancy of monolayer $NbSe_2$. Side-view and top-view of atomic model structures of H_2O (E, F) and O_2 (G, H) adsorbed on dual Se vacancies of monolayer $NbSe_2$. Note: No E_{ads} in case of O_2 (G, H) adsorbed on dual Se vacancies of monolayer $NbSe_2$, due to O_2 is directly dissociated and be embedded in $NbSe_2$.

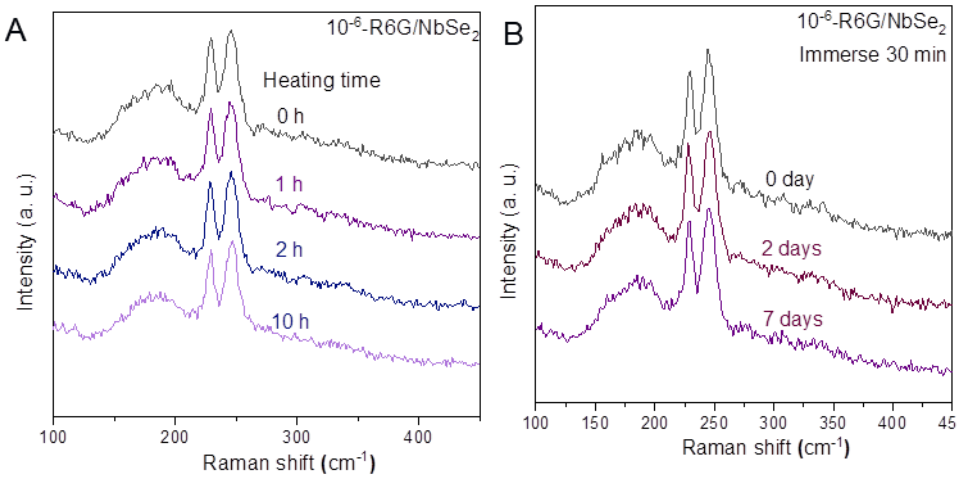

Figure S15. Stable SERS effect of NC-$NbSe_2$ film. (A) The time-dependent evolution of Raman spectra of NC-$NbSe_2$ films exposure to air at 50 °C. (B) The time-dependent evolution of Raman spectra $NbSe_2$ films after being pre-immersed in water for 30 minutes.

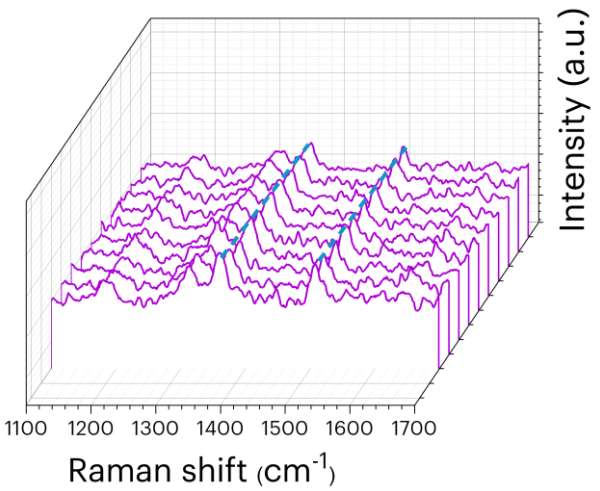

Figure S16. Homogenous SERS performance of as-grown 4-inch NC-$NbSe_2$ film. Raman spectra at 10 different locations randomly distributed in the 10^{-6} M R6G coated 4-inch as-grown NC-$NbSe_2$ film.

Table 1: Comparative Analysis with representative 2D SERS Substrates.

Catalysts	**Dyes**	**Detect Limit (M)**	**Stability**	**Refs.**
Graphene quantum dots	R6G	1×10^{-9}	/	Nature Communications, 2018, 9, 193-202.[1]
1T′-W(Mo)Te_2	R6G	1×10^{-15}	Stable in air with 12 days	*J. Am. Chem. Soc., 2018, 140, 8696-8704.[2]*
NbS_2	MB	1×10^{-14}	Stable in air with 3 days	ACS Nano 2019, 13, 8312-8319.[3]
6L $NbSe_2$	R6G	1×10^{-16}	Unstable SERS in air	J. Mater. Chem. A, 2021, 9, 2725–2733.[4]
$TaSe_2$ Film	R6G	1×10^{-10}	/	*Small 2022, 18, 2107027.[5]*
NC-$NbSe_2$	**R6G**	**1×10^{-10}**	**Stable with 7 days after pre-treatment in water 30 min/ Stable in air with 30 days**	**This work**