Electronic Supplementary Information for "Dependence of Coupling of Quasi 2-D MoS_2 with Substrate on substrate type, Probed by Temperature Dependent Raman Scattering"

Liqin Su,[1] Yong Zhang,[1] Yifei Yu,[2] and Linyou Cao[2]

[1] Electrical and Computer Engineering Department, University of North Carolina at Charlotte, Charlotte, NC 28223, USA.

[2] Department of Materials Science and Engineering, North Carolina State University, Raleigh, NC 27695, USA.

In additional to the sample (1L-ME-SiO_2) used in the main text, two other mechanically exfoliated 1L MoS_2 samples on SiO_2/Si substrate were also studied (labeled as 1L-ME-SiO_2-No2 and 1L-ME-SiO_2-No3), yielding qualitatively very similar results. Figures S1 and S2, respectively, show the optical image, Raman spectrum, Frequency difference between E_{2g}^1 and A_{1g} modes, and temperature dependence of Raman frequency and FWHM (Full Width at Half Maximum) of E_{2g}^1 and A_{1g} modes for these two samples.

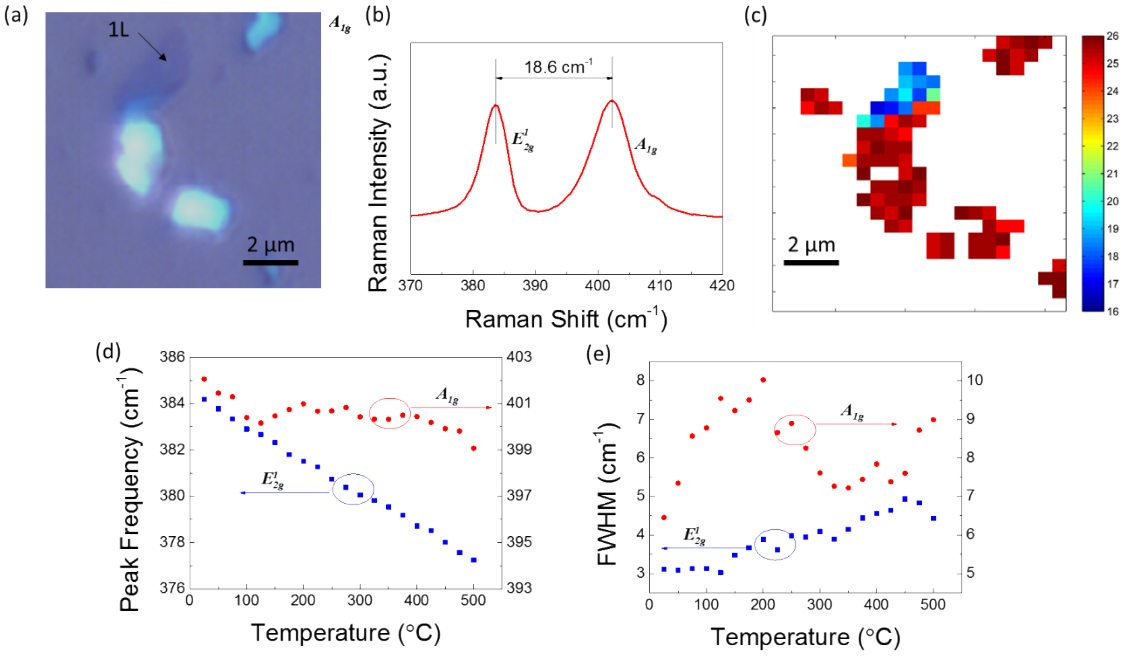

Figure S1. 1L-ME-SiO_2-No2. (a) Optical image of a few flakes of MoS_2 with different thickness, including the one named as 1L-ME-SiO_2-No2. (b) A Raman spectrum of 1L-ME-SiO_2-No2, with the frequency difference between E_{2g}^1 and A_{1g} being 18.6 cm^{-1} (indicating single layer). (c) Map of Raman frequency difference between E_{2g}^1 and A_{1g} modes for all the pieces. (d) and (e) Temperature dependence of Raman frequency and FWHM for E_{2g}^1 and A_{1g} in 1L-ME-SiO_2-No2.

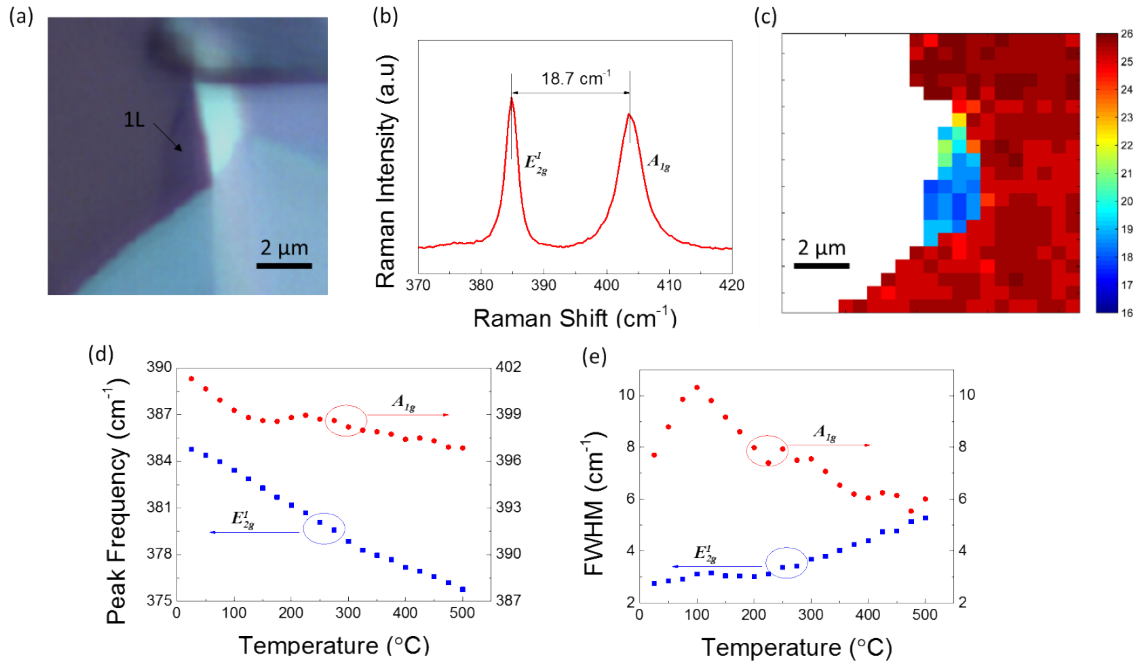

Figure S2. 1L-ME-SiO_2-No3. (a) Optical image of a large piece of MoS_2 with one portion being 1ML thick, named as 1L-ME-SiO_2-No3. (b) A Raman spectrum of 1L-ME-SiO_2-No3, with the frequency difference between E^1_{2g} and A_{1g} being 18.6 cm^{-1} (indicating single layer). (c) Map of Raman frequency difference between E^1_{2g} and A_{1g} modes for all the pieces. (d) and (e) Temperature dependence of Raman frequency and FWHM for E^1_{2g} and A_{1g} in 1L-ME-SiO_2-No3.

The Raman spectra, as well as the maps of Raman frequency difference between E^1_{2g} and A_{1g} modes, of both samples indicate that they are single-layer MoS2 films. Raman mappings were carried out for both samples at room temperature, showing that at single-layer area the Raman frequency variation of A_{1g} mode is greater than that of E^1_{2g} mode, which further confirms that A_{1g} mode is more sensitive to the film morphology variation that was introduced during pressing down the exfoliated thin-film. The temperature dependences of both E^1_{2g} and A_{1g} modes were performed in the temperature range from room temperature (25 °C) to 500 °C (Figure S1(d) and S2(d)). The E^1_{2g} mode exhibits a

close to linear temperature dependence with increasing temperature, while the A_{1g} mode shows strong nonlinearity, which is consistent with sample 1L-ME-SiO_2. The nonlinear temperature dependence of A_{1g} mode is attributed to the morphology changes such as the wrinkles and ripples with increasing temperature. The first-order temperature coefficients of the E_{2g}^1 and A_{1g} modes are -0.0182 ± 0.0013 cm^{-1}/K and -0.0240 ± 0.0048 cm^{-1}/K for 1L-ME-SiO_2-No2 sample, and -0.0170 ± 0.0019 cm^{-1}/K and -0.0310 ± 0.0050 cm^{-1}/K for 1L-ME-SiO_2-No3 sample, respectively. These values are also in a good agreement with the results in the main text for 1L-ME-SiO_2. Furthermore, the temperature dependence of FWHM of the E_{2g}^1 mode is also more linear than the A_{1g} mode for both samples (Figure S1(e) and S2(e)).