Electronic Supplementary Material (ESI) for Nanoscale.

Passivating 1T'-$MoTe_2$ Multilayers at Elevated Temperatures by Encapsulation

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Supplementary Information

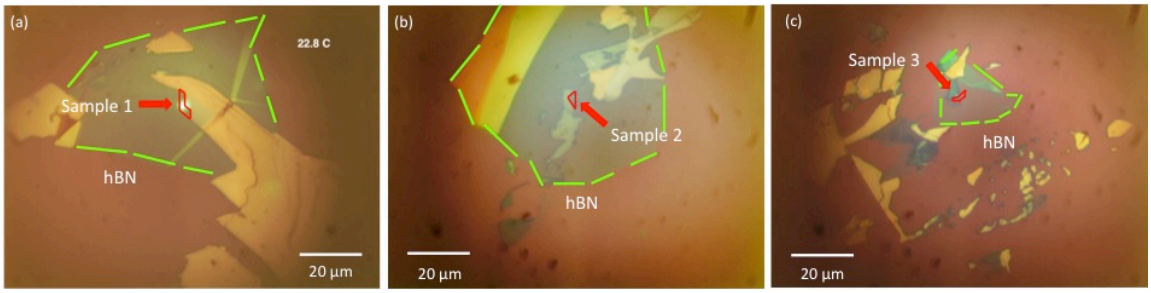

Fig. S1. Optical micrographs of (a) Sample 1, (b) Sample 2, and (c) Sample 3, at room temperature, before heating. Red outlines denoting the thinnest region of the flake, which is probed by Raman scattering, and green outlines denoting the edges of the encapsulating hBN.

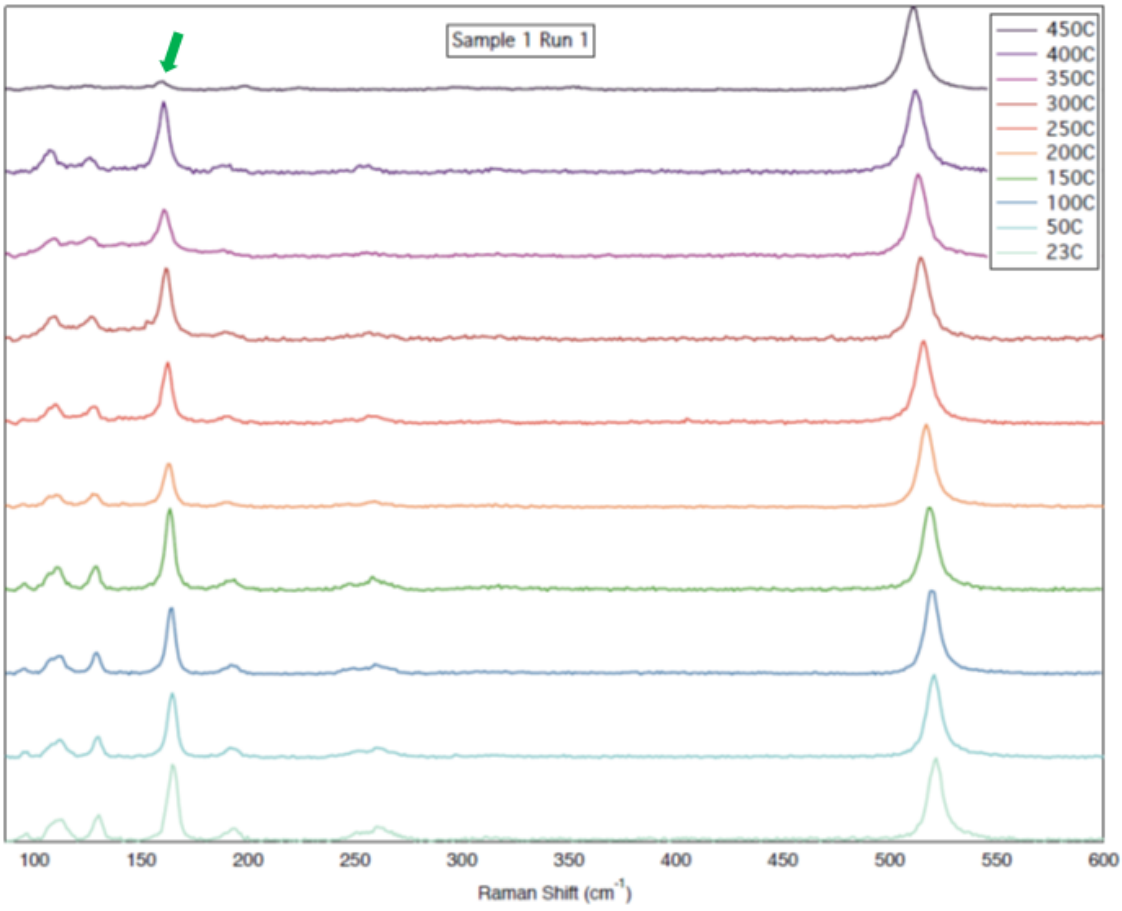

Fig. S2. Raman spectra of encapsulated 1T'-$MoTe_2$ at various temperatures for Sample 1, Run 1 (in air). The green arrow points to position of the strongest initial $MoTe_2$ peak at room temperature, ~164 cm^{-1}.

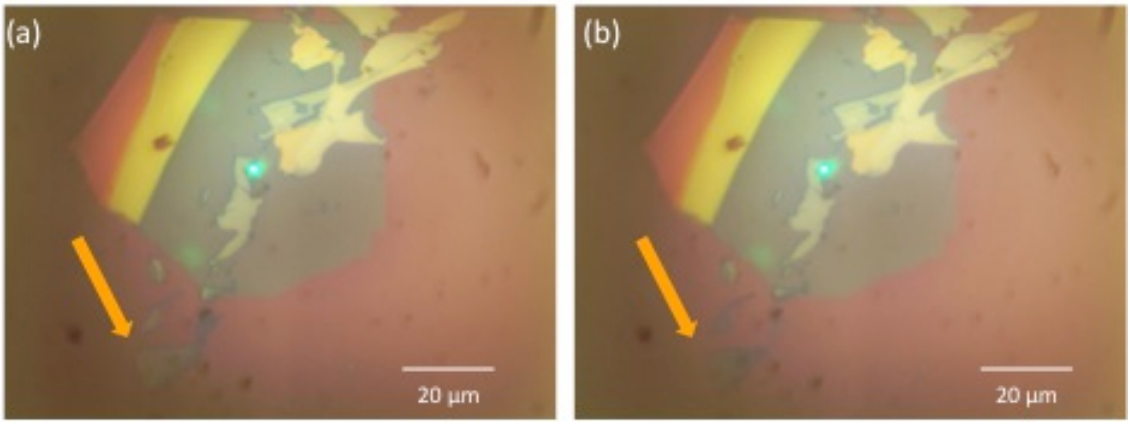

Fig. S3. Optical micrographs of Sample 2 during Run 2 at (a) 250 °C and (b) 300 °C. The orange arrows indicate the decomposition of small, uncovered flakes under and to the left of the sample in this temperature range.

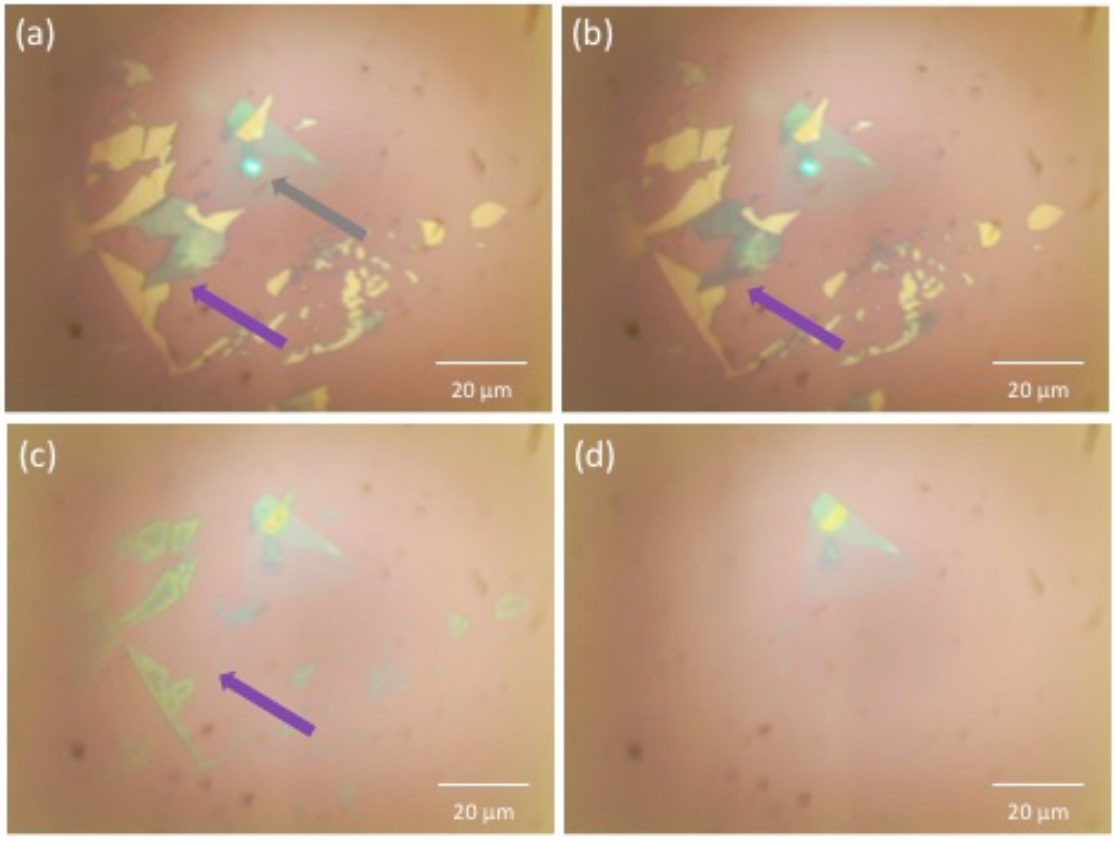

Fig. S4. Optical micrographs of Sample 3, Run 2 at (a) 250 °C, (b) 300 °C, and then after (c) 375 °C and (d) 400 °C, both taken at 100 °C. The gray arrow in (a) indicates where the sample was probed at all temperatures while the purple arrows in (a), (b), and (c) show the decomposition of small, uncovered flakes below and to the left of the sample, which is complete in (d).

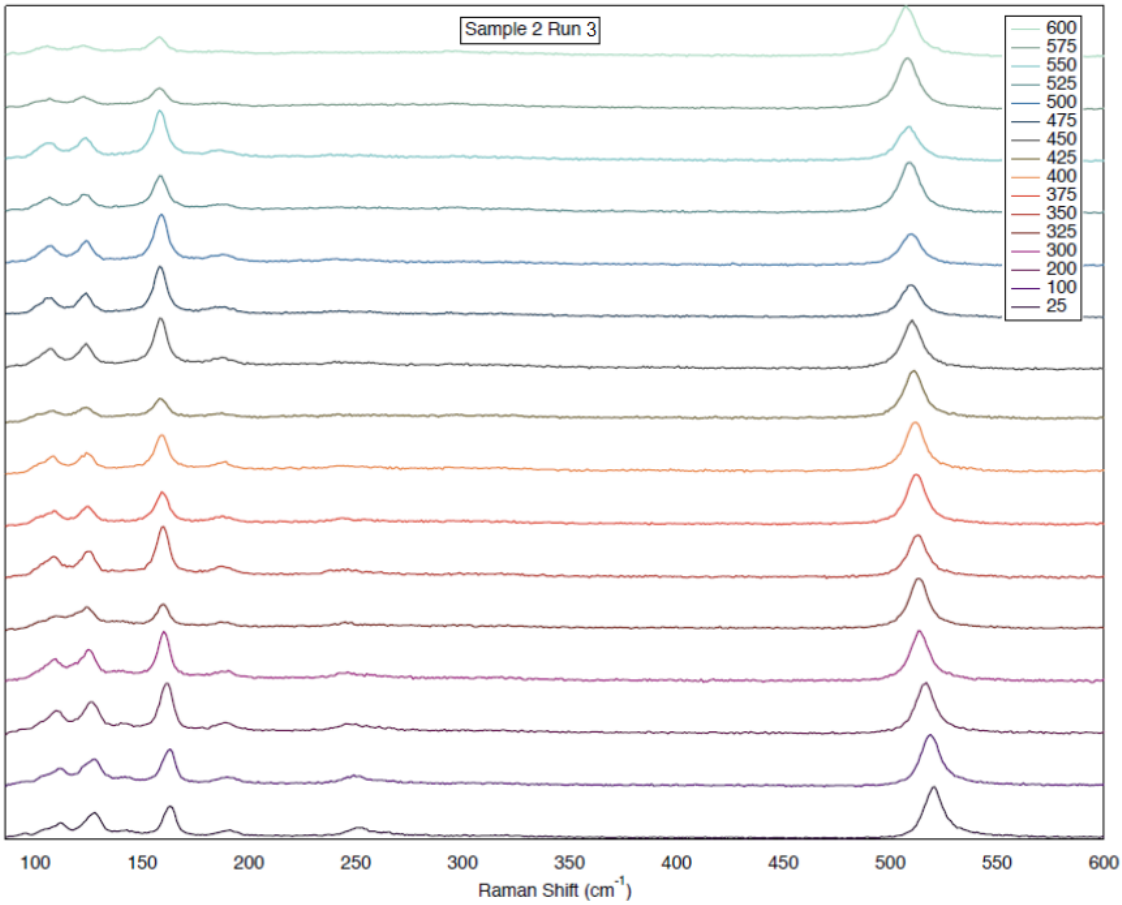

Fig. S5. Raman spectra of encapsulated 1T'-$MoTe_2$ at various temperatures for Sample 2, Run 3 (Ar flow).

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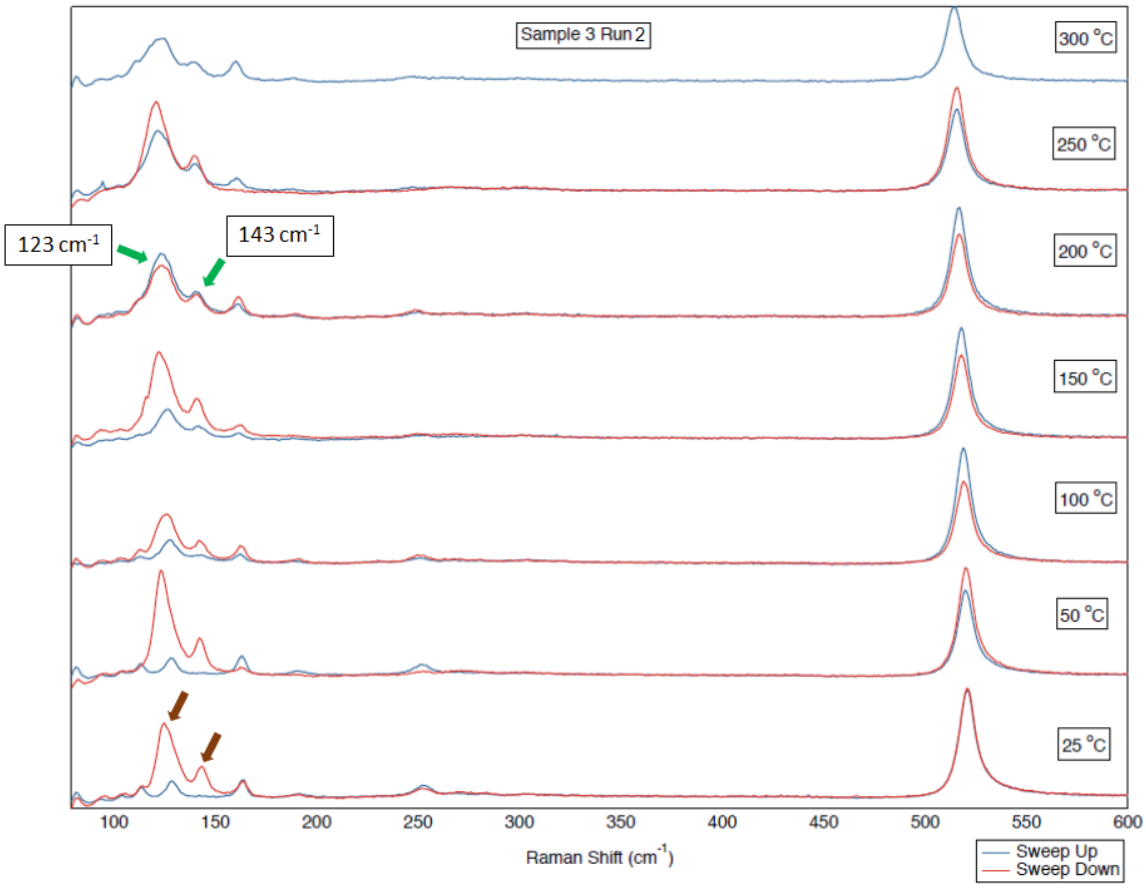

Fig. S6. Raman spectra of encapsulated 1T'-$MoTe_2$ at various temperatures for Sample 3, Run 2 (Ar flow).

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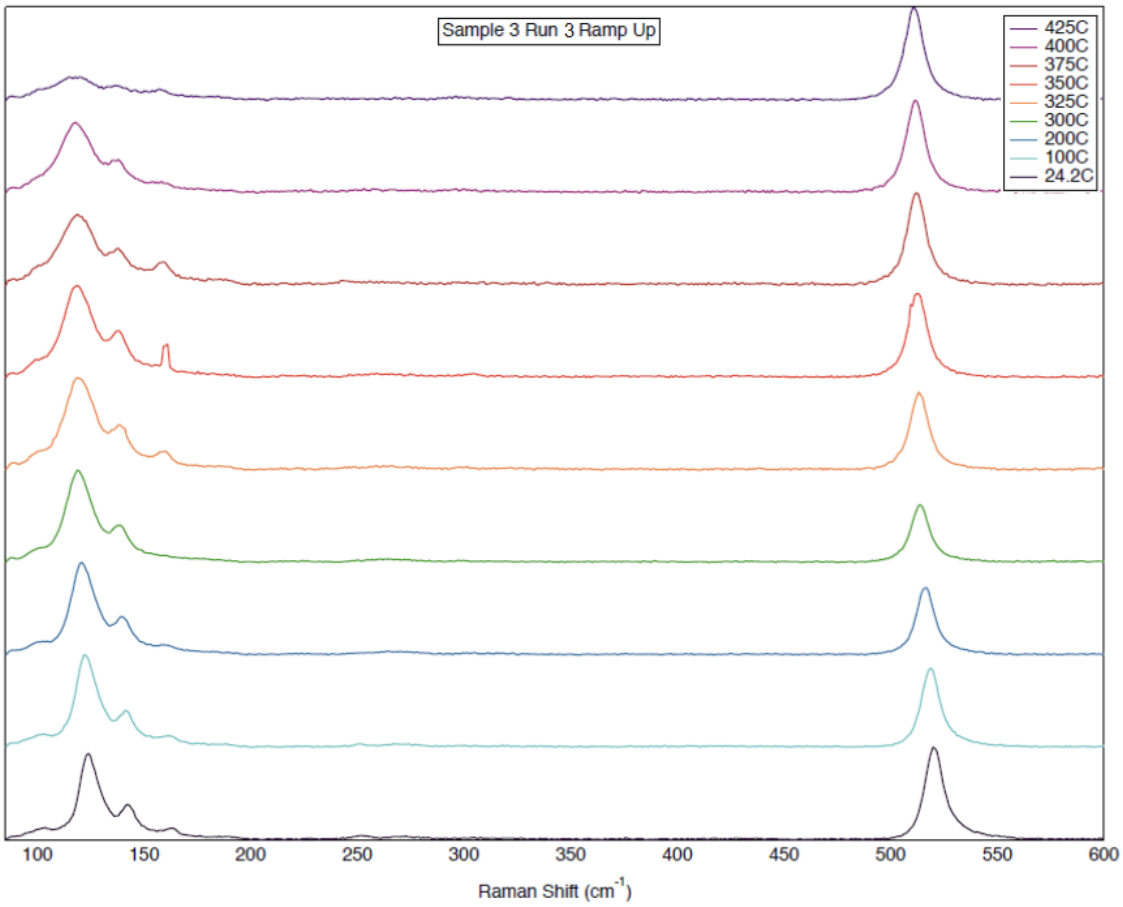

Fig. S7. Raman spectra of encapsulated 1T'-$MoTe_2$ at various temperatures for Sample 3, Run 3 (Ar flow). No $MoTe_2$ Raman signal was observed at and above 450 °C.

Table S1. $MoTe_2$ flake properties for each sample

Sample Number	**$MoTe_2$ Flake Properties**
Sample 1 (on first chip)	9 nm (~6 unit cells) covered by 13 nm (~40 layers) hBN
Sample 2 (on second chip)	4-5 nm (~3 unit cells) covered by 10 nm (~35 layers) hBN
Sample 3 (on second chip)	4 nm (~3 unit cells) covered by 5 nm (~16 layers) hBN

Table S2. Experimental conditions for each sample/run.

Sample and Run Number	**Gas**	**Temperature Heating Sequence**
Sample 1, Run 1	Ambient air	23, 50, 100, 150, 200, 250, 300, 350, 400, 450°C
Sample 2, Run 2	Ar flow	25, 50, 100, 150, 200, 250, 300, 250, 200, 150, 100, 50, 25°C
Sample 2, Run 3	Ar flow	25, 100, 200, 300, 100, 325, 100, 350, 100, …, 600, 100°C
Sample 3, Run 2	Ar flow	25, 50, 100, 150, 200, 250, 300, 250, 200, 150, 100, 50, 25°C
Sample 3, Run 3	Ar flow	24.2, 100, 200, 300, 100, 325, 100, 350, 100, 375, 100, 400, 100, 425°C

Table S3. Fits of frequency vs. temperature for two 1T'-$MoTe_2$ Raman peaks, for Sample 2.

<u>128 cm^{-1} peak</u>

- Run 2 Up: 132.97 (± 0.14) cm^{-1} – [0.013097 (± 0.000321) cm^{-1}/K] T(K)
- Run 2 Down: 130.96 (± 0.13) cm^{-1} – [0.009780 (± 0.000314) cm^{-1}/K] T(K)
- Run 3 Up: 130.31 (± 0.12) cm^{-1} – [0.008400 (± 0.000190) cm^{-1}/K] T(K)
- Run 3 Up, Calibrated: 131.22 (± 0.12) cm^{-1} – [0.010388 (± 0.000190) cm^{-1}/K] T(K)
- Unweighted Average of [Run 2 Up/Down and Run 3 Up, Calibrated]: 131.72 (± 0.13) cm^{-1} – [0.011088 (± 0.000282) cm^{-1}/K] T(K)
- Weighted Average of [Run 2 Up/Down and Run 3 Up, Calibrated]: 131.59 (± 0.13) cm^{-1} – [0.010916 (± 0.000255) cm^{-1}/K] T(K)
- Direct fit of [Run 2 Up/Down and Run 3 Up, Calibrated]: 131.81 (± 0.08) cm^{-1} – [0.0112249 (± 0.000143) cm^{-1}/K] T(K)

<u>164 cm^{-1} peak</u>

- Run 2 Up: 166.78 (± 0.06) cm^{-1} – [0.010200 (± 0.000143) cm^{-1}/K] T(K)
- Run 2 Down: 167.26 (± 0.07) cm^{-1} – [0.011337 (± 0.000148) cm^{-1}/K] T(K)
- Run 3 Up: 166.07 (± 0.058) cm^{-1} – [0.009249 (± 0.000089) cm^{-1}/K] T(K)
- Run 3 Up, Calibrated: 167.19 (± 0.06) cm^{-1} – [0.011581 (± 0.000089) cm^{-1}/K] T(K)
- Unweighted Average of [Run 2 Up/Down and Run 3 Up, Calibrated]: 167.08 (± 0.06) cm^{-1} – [0.011039 (± 0.000525) cm^{-1}/K] T(K)
- Weighted Average of [Run 2 Up/Down and Run 3 Up, Calibrated]: 167.11 (± 0.06) cm^{-1} – [0.011197 (± 0.000665) cm^{-1}/K] T(K)
- Direct fit of [Run 2 Up/Down and Run 3 Up, Calibrated]: 167.50 (± 0.04 cm^{-1}) – [0.011842 (± 0.000066) cm^{-1}/K] T(K)