ESI for

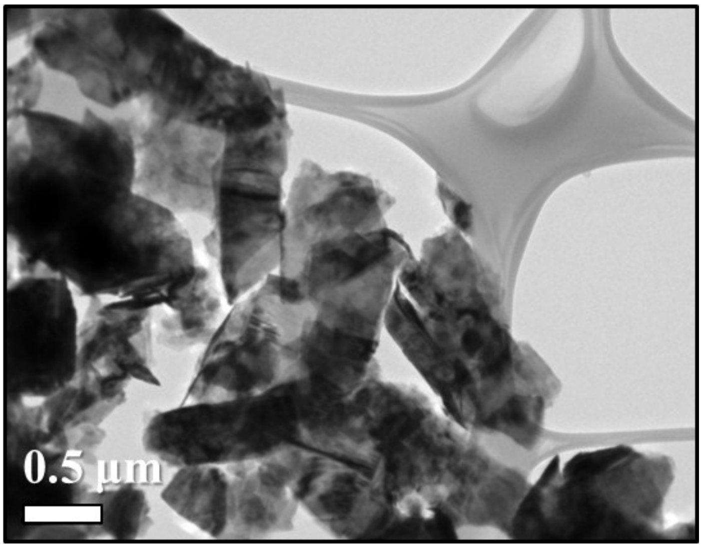
Highly efficient Hydrogen evolution reaction by strain and phase engineering in composites of Pt and MoS_2 nano-scrolls

Da Young Hwang[†], *Kyoung Hwan Choi*[†], *Jeong Eon Park*[†] and *Dong Hack Suh*[†*]

[†]Division of Chemical Engineering, College of Engineering, Hanyang University, Seoul, 04763, Republic of Korea

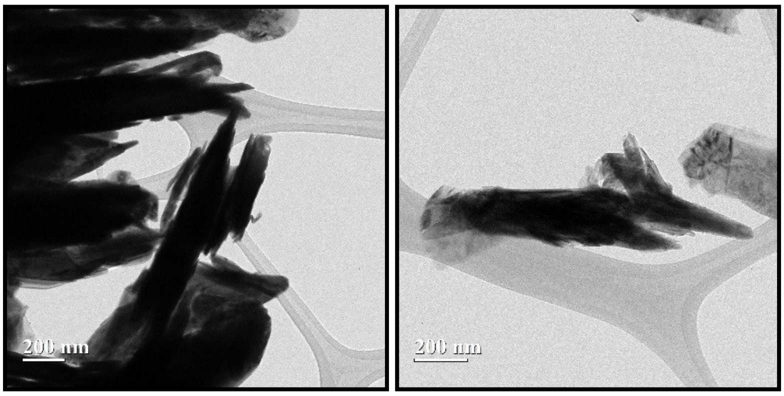
[*]Corresponding author. E-mail: dhsuh@hanyang.ac.kr

Figure S1. TEM images of the dispersed MoS_2 sheets.



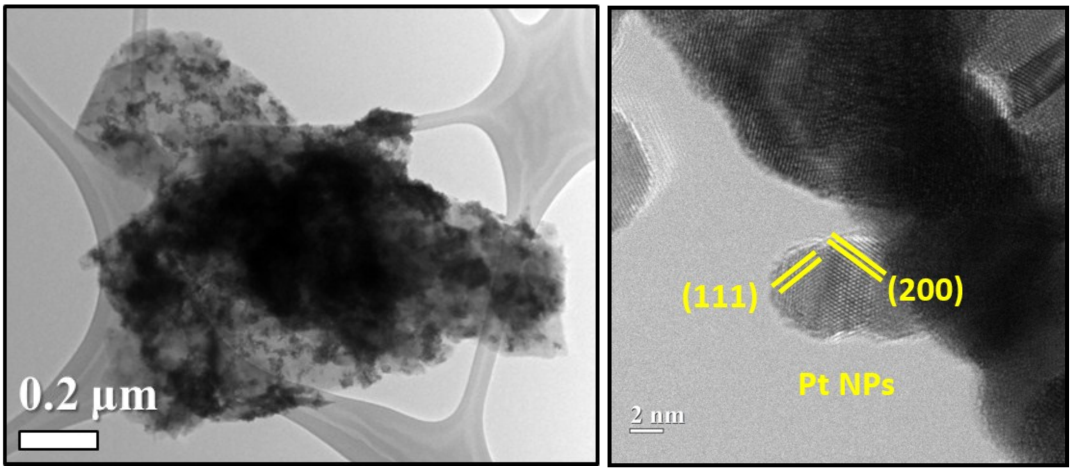
The concentration of the final exfoliated MoS_2 was measured by using the vacuum filter through a weighed membrane. The multi-layer MoS_2 with size of typically several hundred nanometers is observed.

Figure S2. TEM images of MoS_2 scrolls with a low magnification.



The tube-like morphology scrolled by interaction of MoS_2 with LCAs. The TEM images at a low magnification represent the produced MoS_2 scrolls. TEM images of the synthesized MoS_2 scrolls with the continuously increasing vertical distance along an axis.

Figure S3. TEM images of MoS_2@Pt sheets produced by the attachment of Pt NPs to the MoS_2 surface.



TEM images of the synthesized MoS_2@Pt sheets with low magnification. Magnified TEM images of the few layer MoS_2 surface with homogeneous attachment of Pt nanoparticles with size of 3 nm. HR-TEM images of Pt NPs on MoS_2 surface with a corresponding lattice spacing.

Figure S4. TEM images of MoS_2 scrolls@Pt.

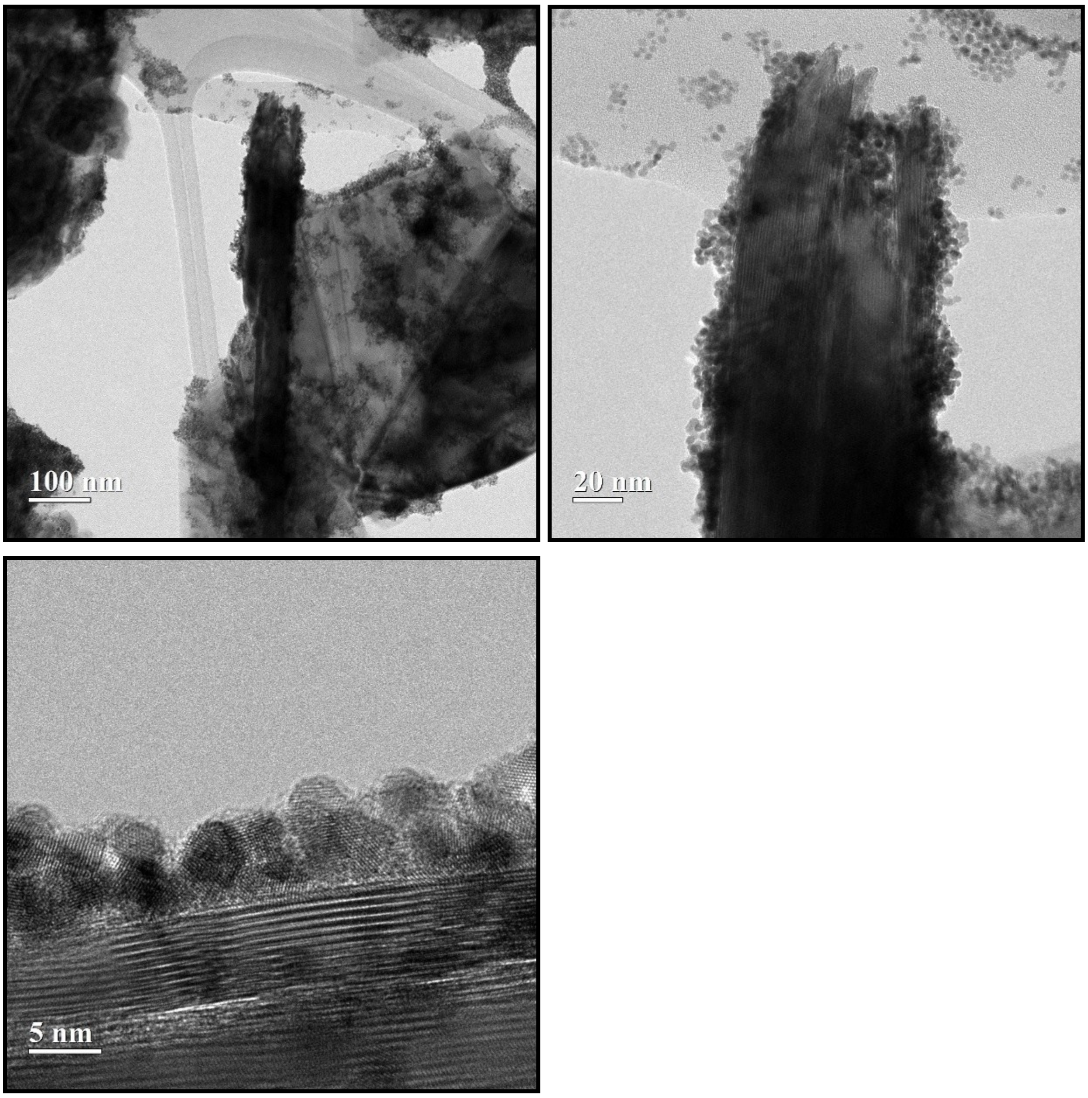
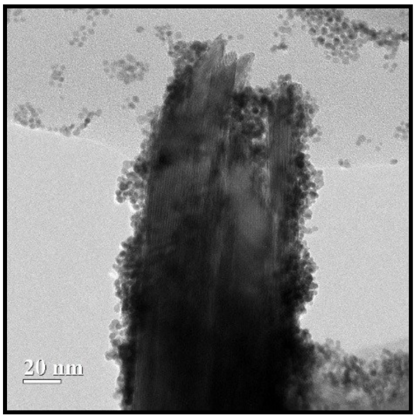


Figure S5. TEM images of MoS_2 scrolls@Pt produced by the attachment of Pt NPs to the MoS_2 scroll surface.



Element	Wt%	Wt% Sigma	Atomic %
S	32.98	1.79	**69.88**
Mo	37.29	2.86	**26.50**
Pt	10.43	0.84	**3.61**
Total:	100.00		**100.00**

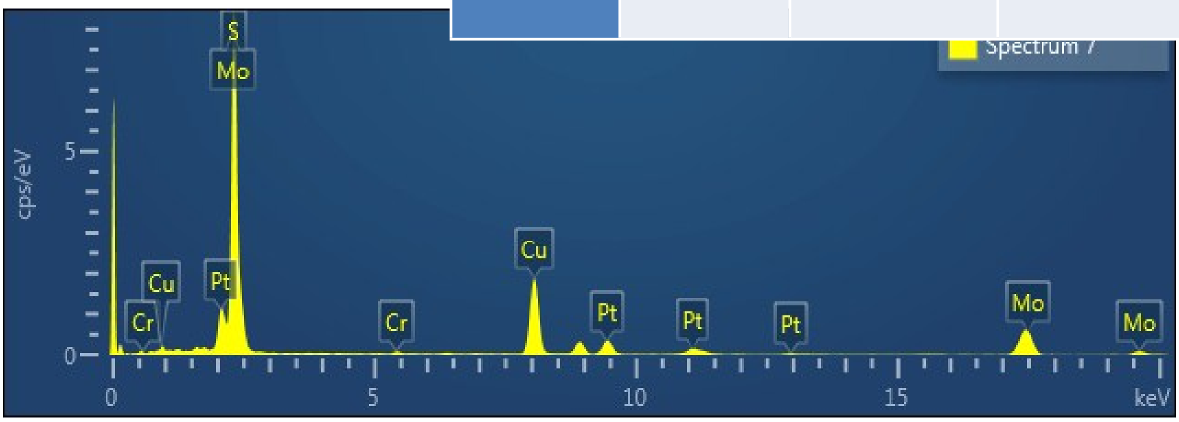


Figure S6. Calculation of the strain energy for MoS_2 derivatives.

We now discuss that the observed behavior can be explained by considering the various MoS_2 derivatives induced uniaxial strain on Raman modes responsible for E^1_{2g} and A_{1g}, correspondingly. The uniaxial strain-induced peak splitting for the E^1_{2g} mode enables us to calculate parameters: the Grüneisen parameter, γ, and the shear deformation potential, β, and the solution of the secular equation for the E_{2g} mode $\Delta\omega_{E_{2g}}$,[1]

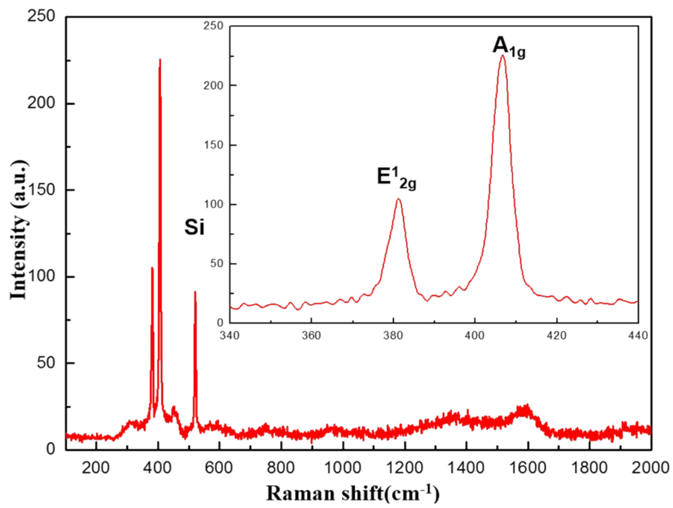
$$\gamma_{E_{2g}} = -\frac{\Delta\omega_{E_{2g}}{}^{+} + \Delta\omega_{E_{2g}}{}^{-}}{2\omega^{0}{}_{E_{2g}}(1-\nu)\varepsilon} \qquad \textbf{(1)}$$

$$\beta_{E_{2g}} = \frac{\Delta\omega_{E_{2g}}{}^{+} - \Delta\omega_{E_{2g}}{}^{-}}{\omega^{0}{}_{E_{2g}}(1+\nu)\varepsilon} \qquad \textbf{(2)}$$

$$\Delta\omega^{\pm}{}_{E_{2g}} = -\omega^{0}{}_{E_{2g}}\gamma_{E_{2g}}(1-\nu)\varepsilon \pm \frac{1}{2}\beta_{E_{2g}}\omega^{0}{}_{E_{2g}}(1+\nu)\varepsilon \qquad \textbf{(3)}$$

Here, Δω is the change of frequency in the Raman mode, $\omega^{0}{}_{E_{2g}}$ is the E_{2g} peak position at zero strain, ν is Poisson's ratio, and ε is the induced uniaxial tensile strain. A Grüneisen parameter of 1.1 and a shear deformation potential of 0.78 for both the monolayer and bilayer MoS_2 attached to a substrate (ν = 0.33) have been reported.[2] In case of formation of MoS_2@Pt scrolls, these calculated parameters are used to estimate the strain applied to a free-standing MoS_2. By inserting $\omega^{0}{}_{E_{2g}}$ = 380.9 cm^{-1} from the Raman spectra, γ_{E2g} = 1.1, β_{E2g} = 0.78, and a Poisson's ratio of ν = 0.27[3] for multilayer MoS_2 in Equation 3, we obtained the $E^1_{2g}{}^{-}$ peak shifts for $\partial\omega_{E_{2g}}{}^{-}/\partial\varepsilon$ with an ~4.9 cm^{-1}/% strain, and the $E^1_{2g}{}^{+}$ peak shifts for $\partial\omega_{E_{2g}}{}^{+}/\partial\varepsilon$ with an ~1.1 cm^{-1}/% strain. These results are nearly equal to the DFT calculated tensile strain on the monolayer MoS_2 with the E^1_{2g}- peak shifts having a strain of 4.5 cm^{-1} /%[4] and the straining monolayer and bilayer MoS_2 with strains of 4.5 ± 0.3 cm^{-1} /% and 4.6 ± 0.4 cm^{-1} /%, respectively.[2]

Figure S7. Raman spectra of the MoS_2 sheets located at 380.9 and 406.4 cm^{-1} with FWHMs of 4.6 and 5.0 cm^{-1}, respectively.



The corresponding bands for MoS_2 sheets are located at 380.9 and 406.4 cm^{-1} with FWHMs of 4.6 and 5.0 cm^{-1}, respectively. The E^1_{2g} mode involves in-plane displacement and shear force of Mo and S atoms, whereas the A_{1g} mode involves out-of-plane symmetric displacement and compressive force of S atoms along the c axis.

References

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