# Supporting Information

## An $MoS_2$/PEDOT: PSS-based flexible NIR-responsive Soft actuator

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## Supporting Figures

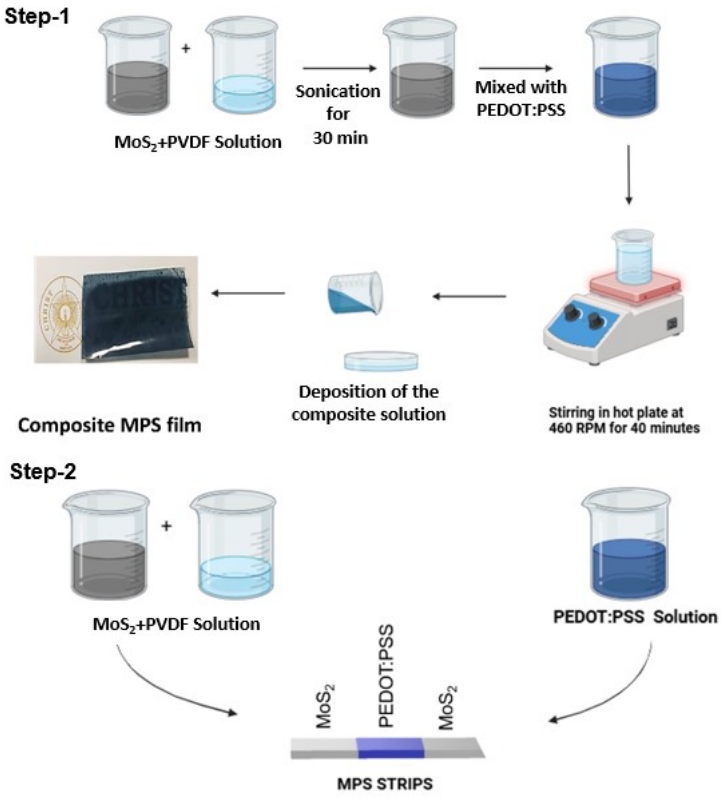


**Figure S1.** Synthesis and fabrication of MPS film with different design.

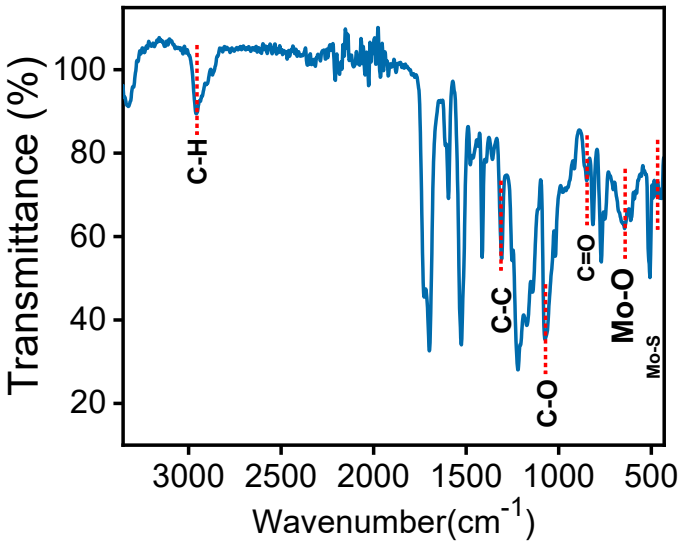


**Figure S2.** FTIR spectra of the MPS film.

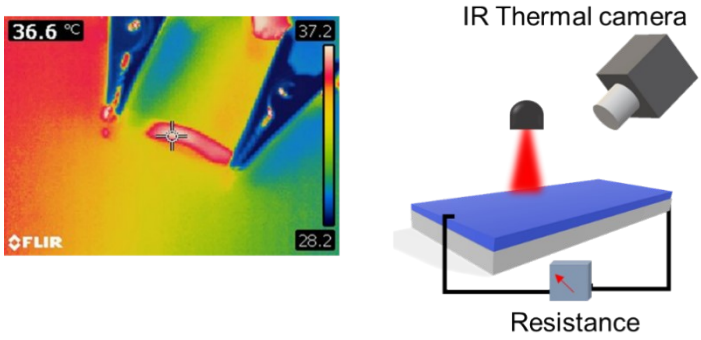


**Figure S3.** Thermal image of the film under IR light exposure. Schematic presentation of measurement of surface resistance under IR light exposure.

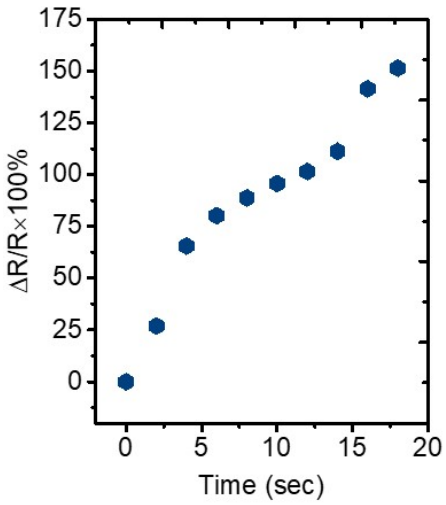


**Figure S4.** Variation of resistance under NIR light exposure

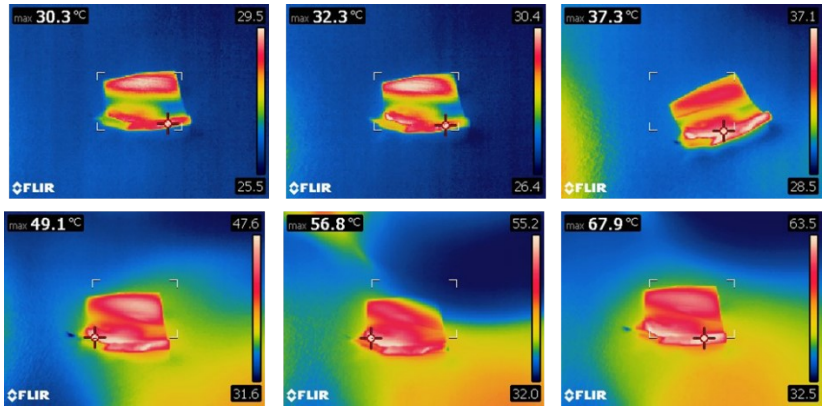


**Figure S5**. Thermal images of the film under NIR light exposure for 20 sec.

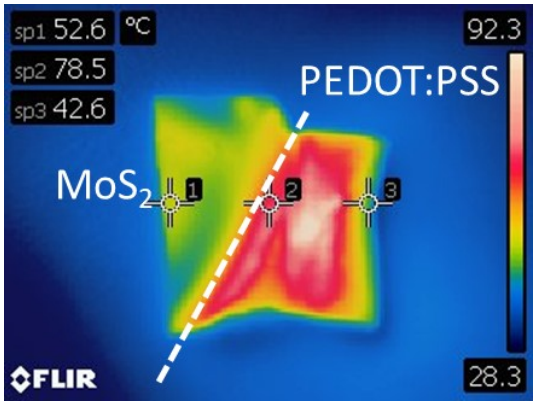


**Figure S6**. Thermal image of strips MPS film

The thermal image of the stripe MPS film taken when exposed to NIR light. It is also important to note that when exposed to NIR light, the only $MoS_2$ film shows no bending. The temperature rises and the actuation of the MPS film changes with increasing light intensity.

**Supporting Discussions:**

**Computational details**

Ground state electronic structure calculations in gas phase of the complexes have been carried out using DFT [1] method associated with the conductor-like polarizable continuum model (CPCM). [2] Becke's hybrid function [3] with the Lee-Yang-Parr (LYP) correlation function [4] was used for the study. The absorbance spectral properties for PDOT with Mo were calculated by time-dependent density functional theory (TDDFT) [5] associated with the conductor-like polarizable continuum model and we computed the lowest 40 singlet– singlet transition. For H atoms we used 6-31+(g) basis set; for C, N, O, Mo atoms we employed LanL2DZ as basis set for all the calculations. The calculated electron-density plots for frontier molecular orbitals were prepared by using Gauss View 5.1 software. All the calculations were performed with the Gaussian 09W software package. [6] Gauss Sum 2.1 program [7] was used to calculate the molecular orbital contributions from groups or atoms. Molecular electrostatic potential (MEP) analysis is obtained from the optimised structure using B3LYP/6–31+(g) standard basis set in gas phase.

**FTIR analysis:**

The peaks of $MoS_2$/PEDOT:PSS nanocomposites at 852 $cm^{-1}$, 1068 $cm^{-1}$, 1359 $cm^{-1}$, 1681 $cm^{-1}$ & 3328 $cm^{-1}$ correspond to S-O, C=O, C–C stretching of thiophene ring and O–H functional groups present in PEDOT:PSS respectively [8-9]. The bands at 450$cm^{-1}$, 641 $cm^{-1}$ are attributed to $MoS_2$ is due to Mo-S, Mo-O and S=O bond, peak at 913$cm^{-1}$ is assigned to the aloxy group (C-O). 2921 $cm^{-1}$ are assigned to the C-H stretching of PEDOT and PSS [10].

**Determination of σ:**

For σ measurements,

$R = \rho/A \times L$

Where A is cross sectional area of the sample

conductivity $\sigma = 1/\rho$

The value of ¼ for α that is observed in the graph is the direction can be interpreted using Variable range hopping (VRH) model. In VRH model, the exponents α equals to 1/(d+1), where d is the dimensionality of the electrical conduction path.

**Calculation of energy conversion efficiency:**

The photothermal conversion efficiency was given by

$$\eta = \frac{E_i}{E_o} \times 100\% = \frac{PSt}{\frac{m_0 v_0^2}{2} + m_0 g \Delta h}$$

Where $E_i$ is the input energy which was calculated using formula

$E_i = PSt$

$P$ is the light power = 300 W/$cm^2$

$S$ is the light facula area= 0.84 $cm^2$

$t$ is the irradiation time = 2s

The total input energy $E_i$ is the input energy = $4.18 \times 10^{-4}$ J

Where $E_o$ is the output energy which was calculated using formula

$$E_o = \frac{m_0 v_0^2}{2} + m_0 g \Delta h$$

$V_o$ is the maximum speed density during uplift = $0.075 \times 10^{-2}$ m/s. $\Delta h$ is the lifting distance where the object showed the maximum speed =8.3 mm. $m_o$ is the weight of the object = 14.4mg

The total out energy $E_o$ is = $0.0863 \times 10^{-2}$

The total conversion efficiency is $\eta = \frac{E_i}{E_o} \times 100\% = 20\%$

**Table S1:** Comparison of actuation property of different sample under NIR exposure

| **Materials** | **Actuation time** | **Efficiency** | **Displacement/bending angle** | **Reference** |
|---|---|---|---|---|
| $MoO_2$/PNIPAM | 25 s | 62% | 15 mm | [11] |
| $MoS_2$ nanoflower And nanosheets | NA s | 13.77% and 25.68% | NA | [12] |
| $WSe_2$/Graphene nanosheets | 1 s | ~39% | 11 mm | [13] |
| GO/BOPP | 4 s | NA | 1.5 cm ( bending curvature) | [14] |
| $MoS_2$/PEDOT:PSS | ~2-3 sec | 20% | 8.3 mm | Current work |

**Table S2:** Comparison of actuation property and other experimental parameters of different 2D sample under NIR exposure.

| **Material** | **NIR wavelength (nm)** | **Actuation Mechanism** | **Response Time** | **References** |
|---|---|---|---|---|
| $MoTe_2$ | 980- 1064 | Thermally triggered | Slow Moderate | [15] |
| $MoS_2$- Graphene | 808 | Photothermal | ~2s | [16] |
| Mxene($Ti_3CT_x$) | 808 | Photothermal bending swelling | < 5s | [17] |
| Graphene Oxide | 808-980 | Photothermal expansion | ~seconds | [18] |
| $MoS_2$/PEDOT:PSS | 650 | Photothermal bending/rolling and twisting | ~2-3 sec | Current work |

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