

Electronic supplementary information

From Tanghulu-like to Cattail-like SiC Nanowire Architectures:

Interfacial Design of Nanocellulose Composites toward Highly Thermal Conductivity

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Shengdu Yang and Bai Xue contributed equally to this work.

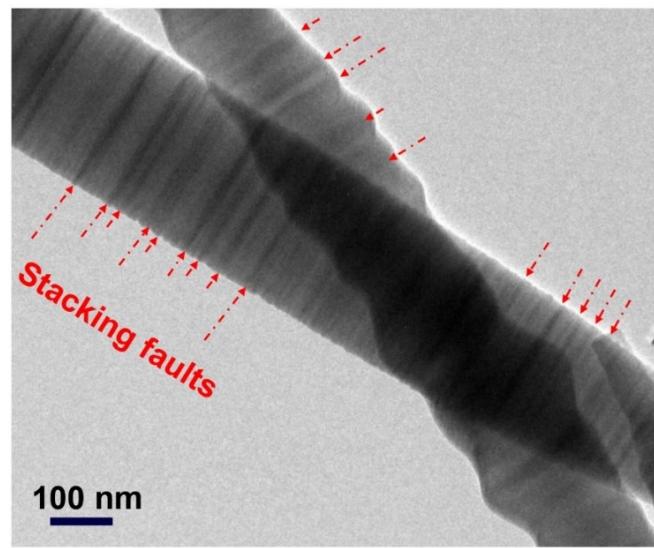


Figure S1. TEM image of the bare SiCNWs

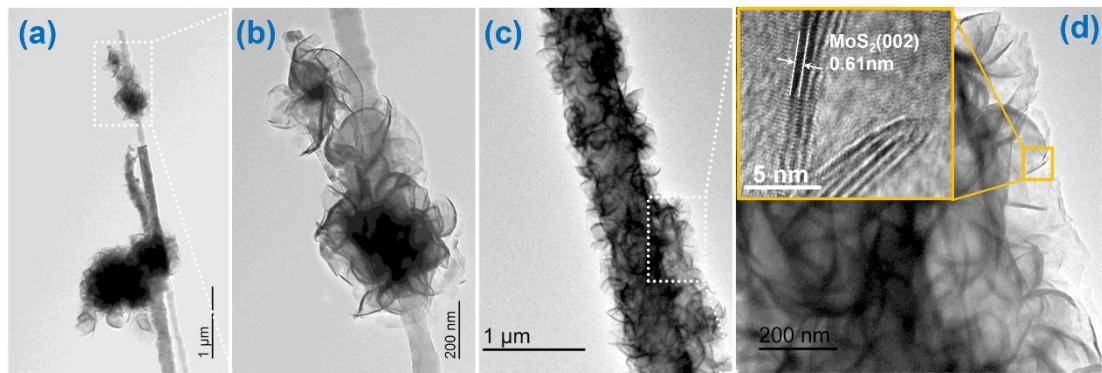


Figure S2: (a) and (b) TEM images of L-MoS₂-SiCNWs. (c) and (d) TEM images of H-MoS₂-SiCNWs.

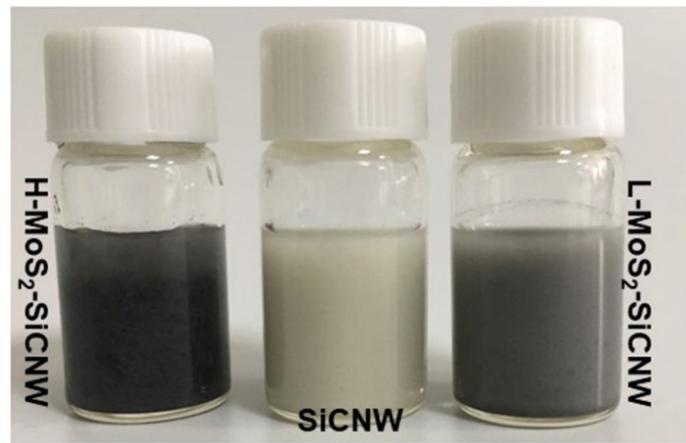


Figure S3. Digital photos showing the dispersion state of synthetic nanohybrids

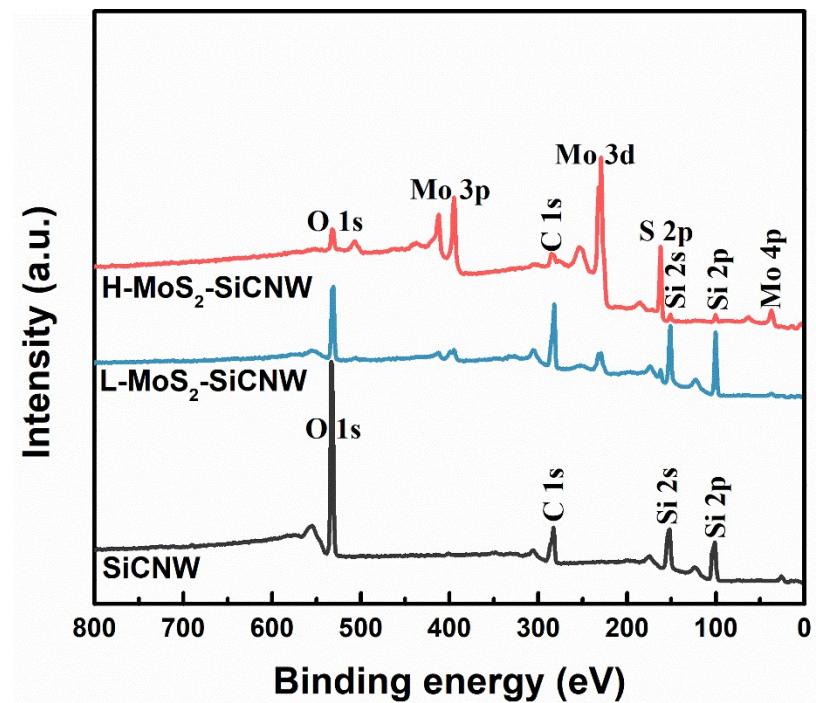


Figure S4: Full-range XPS spectra of bare SiCNW, L-MoS₂-SiCNW, and H-MoS₂-SiCNW hybrids.

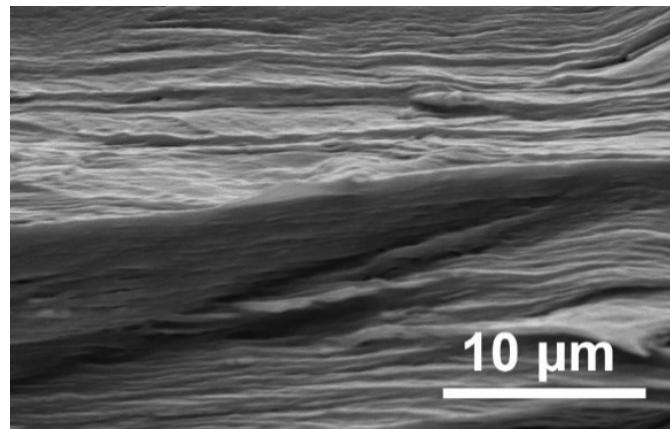


Figure S5: The cross-section SEM image of pure CNF film.

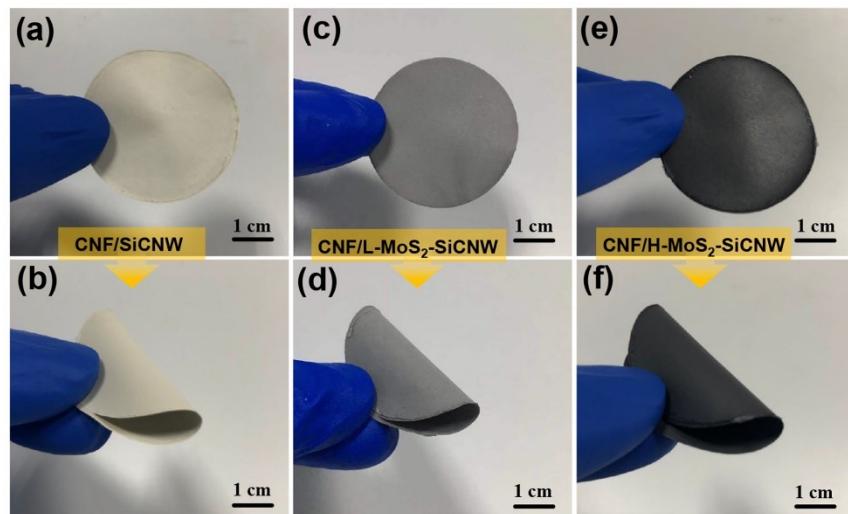


Figure S6: Digital photos of (a, b) CNF/SiCNW, (c, d) CNF/L-MoS₂-SiCNW and (e, f) CNF/H-MoS₂-SiCNW films, respectively.

Table S1: Comparison with TC and TCE values of previously reported composites

Ref.	Fillers	Matrix	Loading (wt%)	TC ($W m^{-1}K^{-1}$)		TCE	Testing way
				TC_{\perp}	$TC_{//}$		
S1	BNNS	Epoxy	~40	◇0.7	◆6.54	3170	Steady-state
S2	PMMA-g-FCNT	PMMA	15	◇~0.35	◆1.16	510	Laser flash
S3	ND	CNF	0.5	◇0.118	◆9.82	775	Laser flash
S4	<i>f</i> BNNS	CNF	70	◇~0.6	◆12.79	699	Laser flash
S5	FCNT	NFC	35	◇0.83	◆14.1	729	Laser flash
S6	MgO@rGO	NFC	20	◇0.32	◆6.17	630	Laser flash
S7	BNNPs	NFC	40	◇~0.5	◆20.64	985	Laser flash
S8	GNP	PDA	44.4	◇0.69	◆13.42	-	Laser flash
S9	rGO	NFC	30	◇0.07	◆6.17	550	Laser flash
S10	CPGO	CNF	70	◇~0.3	◆12.75	165	Laser flash
S11	BNNS@PDA	ANF	50	◇0.62	◆3.94	196	Steady-state
S12	BNNS-OH	CNF	75	◇0.45	◆15	235	Laser flash
This work	H-MoS ₂ -SiCNW	CNF	40 (22.5 vol%)	★0.68	★19.76	1408	Laser flash

According to our defined the rule of mixtures (Eq. (S1)), the thermal conductivity of L/H-MoS₂-SiCNW ($K_{p(mix)}$) can be calculated from,

$$K_{p(mix)} = K_{SiCNW}f + K_{MoS_2}(1 - f) \quad (S1)$$

where $K_{MoS_2}=82 \text{ Wm}^{-1}\text{K}^{-1}$, $K_{SiCNW}=120 \text{ Wm}^{-1}\text{K}^{-1}$ and f is the volume fraction of SiCNW in MoS₂/SiCNW hybrid.

$$\rho_{SiCNW} = 3.21\text{g/cm}^3, \rho_{MoS_2} = 4.80\text{g/cm}^3$$

The exact content of MoS₂ is 78.6 wt% (64.8 vol%) in L-MoS₂-SiCNWs and 97.0 wt% (95.6 vol%) in H-MoS₂-SiCNWs.

Thus, $f=35.2 \text{ vol\%}$ (L-MoS₂-SiCNW), $f=4.4 \text{ vol\%}$ (H-MoS₂-SiCNW)

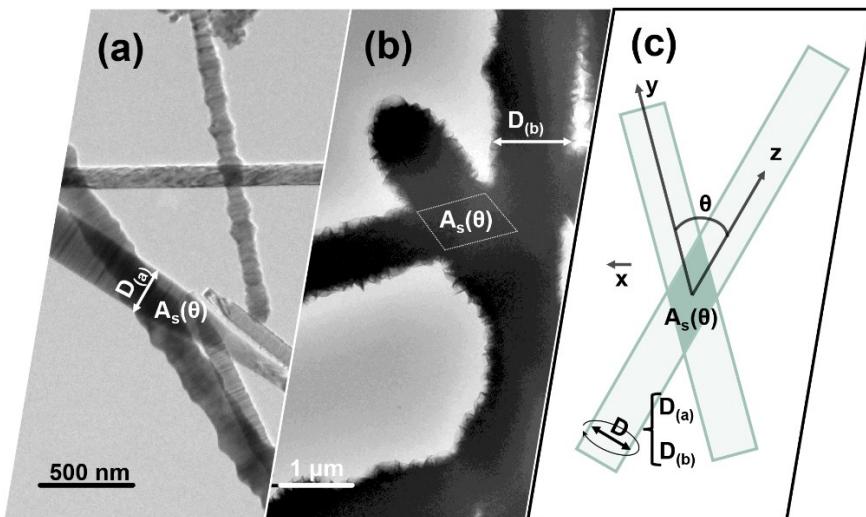


Figure S7: The average overlap area (\bar{A}_s) between adjacent fillers for (a) bare SiCNWs and (b) H-MoS₂-SiCNWs. (c) Schematic diagram of the average overlap area (\bar{A}_s).

$$\bar{A}_s = \frac{2D^2}{\pi} \left[\ln \left(\sin \frac{\theta}{2} \right) - \ln \left(\cos \frac{\theta}{2} \right) \right]_0^{\frac{\pi}{2}} \quad (S2)$$

$$A_{s,c} = \frac{D_{(a,b)}^2}{\sin(\theta_c)} \quad (S3)$$

$$\bar{A}_s = \frac{2D^2}{\pi} \delta(p) \quad (\text{S4})$$

$$\delta(p) = \ln \left[\frac{\sqrt{1+p^{-1}} + \sqrt{1-p^{-1}}}{\sqrt{1+p^{-1}} - \sqrt{1-p^{-1}}} \right] \quad (\text{S5})$$

$\bar{A}_s = 5.46 \times 10^{-14}$ m² for bare SiCNWs and $\bar{A}_s = 3.19 \times 10^{-12}$ m² for H-MoS₂-SiCNWs.

Table S2: The values of V_c , K_o , and $t(p)$ for CNF/SiCNW and CNF/H-MoS₂-SiCNW.

Sample	V_c	K_o	$t(p)$
CNF/SiCNW	8.7×10^{-4}	5.95	0.23
CNF/H-MoS ₂ -SiCNW	8.0×10^{-3}	6.79	0.50

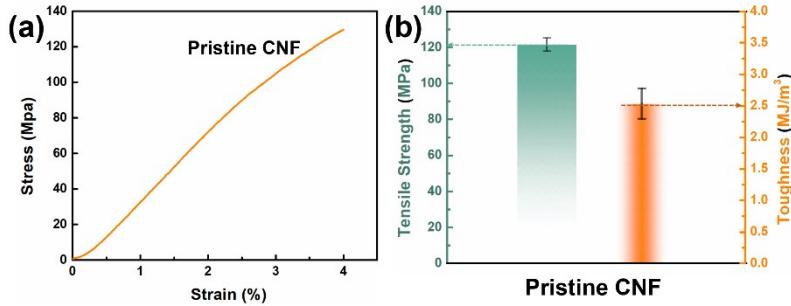


Figure S8. (a) Typical strain-stress curve and (b) Tensile strength and toughness of pure CNF film.

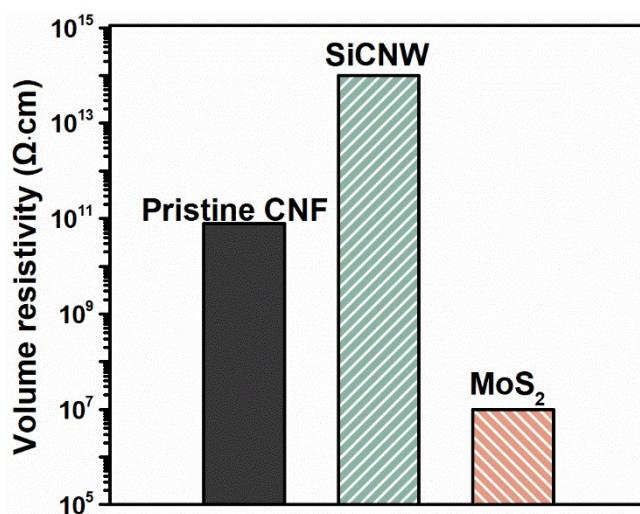


Figure S9. Volume resistivities of Pristine CNF, SiCNW, and MoS₂

As shown in Figure S9, the volume resistance of pure SiCNWs (2.1×10^{14} Ω·cm)

is far higher than that of pure CNF film ($7.9 \times 10^{10} \Omega \cdot \text{cm}$). Thus, the volume resistance of CNF/SiCNW is largely increased to $2.4 \times 10^{13} \Omega \cdot \text{cm}$ with the introduction of 22.5 vol% SiCNWs. However, the volume resistance of MoS₂ is as low as $1.3 \times 10^7 \Omega \cdot \text{cm}$. Hence, with the introduction of SiCNW hybrids (L-MoS₂-SiCNW and H-MoS₂-SiCNW), the volume resistances of CNF/L-MoS₂-SiCNW and CNF/H-MoS₂-SiCNW are moderately reduced to $1.7 \times 10^{13} \Omega \cdot \text{cm}$ and $4.1 \times 10^{12} \Omega \cdot \text{cm}$, respectively, which is still superior to that of pure CNF film.

References

- S1. J. Han, G. Du, W. Gao and H. Bai, *Adv. Funct. Mater.*, 2019, **29**, 1904c12.
- S2. X. Wang and P. Wu, *Chem. Eng. J.*, 2019, **369**, 272-279.
- S3. N. Song, S. Cui, X. Hou, P. Ding and L. Shi, *ACS Appl. Mater. Interfaces*, 2017, **9**, 40766-40773.
- S4. K. Wu, J. Fang, J. Ma, R. Huang, S. Chai, F. Chen and Q. Fu, *ACS Appl. Mater. Interfaces*, 2017, **9**, 30035-30045.
- S5. X. Wang and P. Wu, *ACS Appl. Mater. Interfaces*, 2018, **10**, 34311-34321.
- S6. M. Ma, L. Xu, L. Qiao, S. Chen, Y. Shi, H. He and X. Wang, *Chem. Eng. J.*, 2019, **385**, 123714.
- S7. Q. Li, Z. Xue, J. Zhao, C. Ao, X. Jia, T. Xia, Q. Wang, X. Deng, W. Zhang and C. Lu, *Chem. Eng. J.*, 2020, **383**, 123101.
- S8. F. Luo, K. Wu, J. Shi, X. Du, X. Li, L. Yang and M. Lu, *J. Mater. Chem. A*, 2017, **5**, 18542-18550.
- S9. N. Song, D. Jiao, P. Ding, S. Cui, S. Tang and L. Shi, *J. Mater. Chem. C*, 2016, **4**,

305-314.

S10. Y. Liu, M. Lu, Z. Hu, L. Liang, J. Shi, X. Huang, M. Lu and K. Wu, *Chem. Eng.*

J., 2019, **383**, 122733.

S11. T. Ma, Y. Zhao, K. Ruan, X. Liu, J. Zhang, Y. Guo, X. Yang, J. Kong and J. Gu,

ACS Appl. Mater. Interfaces, 2020, 12, 1677-1686.

S12. Z. Hu, S. Wang, G. Chen, Q. zhang, K. Wu, J. Shi, L. Liang and M. Lu, *Compos.*

Sci. Technol., 2018, **168**, 287-295.