Insights into Hydroelectric Nanogenerators: Numerical Simulations and Experimental Data Analysis

Materials and Methods.

1.1 Chemicals and Materials

Wool cloth (175.5 g/m^2, 0.29 mm in thickness) was purchased from Nanshan Worsted Woolen Factory, Yantai City, China and cut into stripes (4 × 0.5 cm). Lithium fluoride (LiF), titanium aluminium carbide 312 (Ti_3AlC_2), sodium chloride (NaCl), lithium chloride (LiCl), hexadecyltrimethylammonium bromide (CTAB), urea, lactic acid, and ammonia solution were obtained from Sigma-Aldrich, Australia. All the chemicals were of analytical grade and used as received. KB nanoparticles were obtained from Lion King Co., Japan. Zinc electrode wires (Zn) with a diameter of 0.6 mm were purchased from the local market in Geelong, Australia. A resistor (150 Ω) and a supercapacitor (47 mF, 5.5 VDC) were purchased from Jaycar Electronics, Geelong, Australia. A Milli-Q ultrapure water purification system (Merck) was used to prepare deionized water (DI water) with a resistivity of approximately 1.6×10^{-4} s·m^{-1}.

1.2 Preparation of ink

A KB ink was prepared by dispersing KB powders (10 g) in DI water (1 L) with the assistance of CTAB (20 g) (mass ratio of KB to CTAB was 1:2) under sonication for 4 h. SMX nanosheets were prepared via selectively etching aluminium from Ti_3Al_2C MAX phase with the minimally intensive layer delamination (MILD) method [1-3]. Lithium fluoride (LiF, 0.5 g) was first added to HCl acid (9 M, 10 mL) under stirring. After 5 min, Ti_3AlC_2 powder (0.5 g) was added to the acidic solution and stirred for one day at 35 °C. The resulting solution was centrifuged at 1331 rcf for 10 min, and the precipitate was washed with DI water several times until the pH of the supernatant reached around 6.5. The sediment was dispersed in DI water and centrifuged at 244 rcf for 20 min to remove multilayer MXene sediments, resulting in a dispersion of singlelayer MXene. The obtained SMX was diluted to a concentration of 23 mg/mL as SMX ink and stored in a freezer (-20 ˚C) for subsequent use.

1.3 Preparation of artificial sweat and fabrication of the SMX-based HENGs

To prepare HENGs, the pristine wool stripes (0.5 × 4 cm^2) were treated with a plasma cleaner (John Morris, air plasma) at 64 W for 2 min under 0.05 mbar to improve their hydrophilicity [4]. The wool stripes were then dipped in the SMX, OKB ink or their mixtures in different OKB/SMX ratios for 3 s and dried in a vacuum oven (Binder Vacuum Oven, Model VD 23, 0.9 kW) at 53 ˚C for 2 h. Zn electrodes were then placed on both ends of the coated wool stripes to produce HENGs.

1.4 Analysis and testing procedure of the HENGs

The electrical output performance of the HENGs was analyzed and tested. The negative and positive probes of a digital multimeter (Keysight, 34454A) were connected to the two ends of the devices. Different solutions (DI water, sweat, 0.7, 1.4, 2.1, and 2.8 M NaCl) (40 μL) were pipetted onto one end of the wool stripes (negative electrode). The short-circuit current (I_{SC}), resistance, and open circuit voltage (V_{OC}) were recorded. To obtain high voltages and currents, multiple cloth stripes were connected in series within one device.

Table S1 FEM parameters and their values

Variable	Value [unit]	Description
s_1	-	Water phase
s_2	-	Air phase
W	0.5 [cm]	Length of the meshed domain
H	4 [cm]	Width of the meshed domain
th	0.3 [mm]	Thickness of the meshed domain
γ	3.52 [N/m]	Surface tension

θ	0 °	Water contact angle in HENGs
R_c	8.8 × 10^{-7} [m]	Pore size
p_{ec}	$2\gamma cos\theta/R_c$	Inlet capillary pressure
λ_p	2	Pore size distribution index
ϵ_p	0.6	Porosity
k	$\epsilon_{p/8}*R_{c}{}^\wedge 2$	Permeability
ρ_{water}	1000 [kg·m^{-3}]	Water density
ρ_{air}	1 [kg·m^{-3}]	Air density
μ_{water}	1.002 × 10^{-3} [Pa·s]	Dynamic viscosity of water
μ_{air}	1.76 × 10^{-5} [Pa·s]	Dynamic viscosity of air
ε_0	8.85 × 10^{-12} [F·m^{-1}]	Vacuum permittivity
ε_r	80	Relative permittivity of water
ζ	-45 [mV]	Zeta potential of SMX
σ	485 [μS·cm^{-1}]	Fluidic conductivity
I	$v*\varepsilon_0*\varepsilon_r*\zeta*s_1/\ k*f_{(t)}$	Streaming current
V	$v*\varepsilon_0*\varepsilon_r*\zeta*s_1/\ k*\sigma*f_{(t)}$	Streaming potential
p_{VA}	2.31 × 10^3 [Pa]	Partial pressure of vapor in saturated air at 293.15 K
$p_{VA'}$	$p_{VA}\times RH$	Partial pressure of water vapor in air at given RH
RH	60%	Relative humidity
p_{in}	0 [Pa]	Inlet pressure in the HENG channel
p_{evap}	3.5 × 10^6 [Pa]	Evaporation pressure
p_{out}	$p_{VA'}-p_{ec}*(s_1)^{-\frac{1}{lp}}*step1(s1)-\rho_{air}*H$	Outlet pressure in SMX channel

T	20 [°C]	Temperature
M_{water}	18 [g·mol^{-1}]	Water molar weight
M_{NaCl}	58.44 [g·mol^{-1}]	Molar weight of NaCl

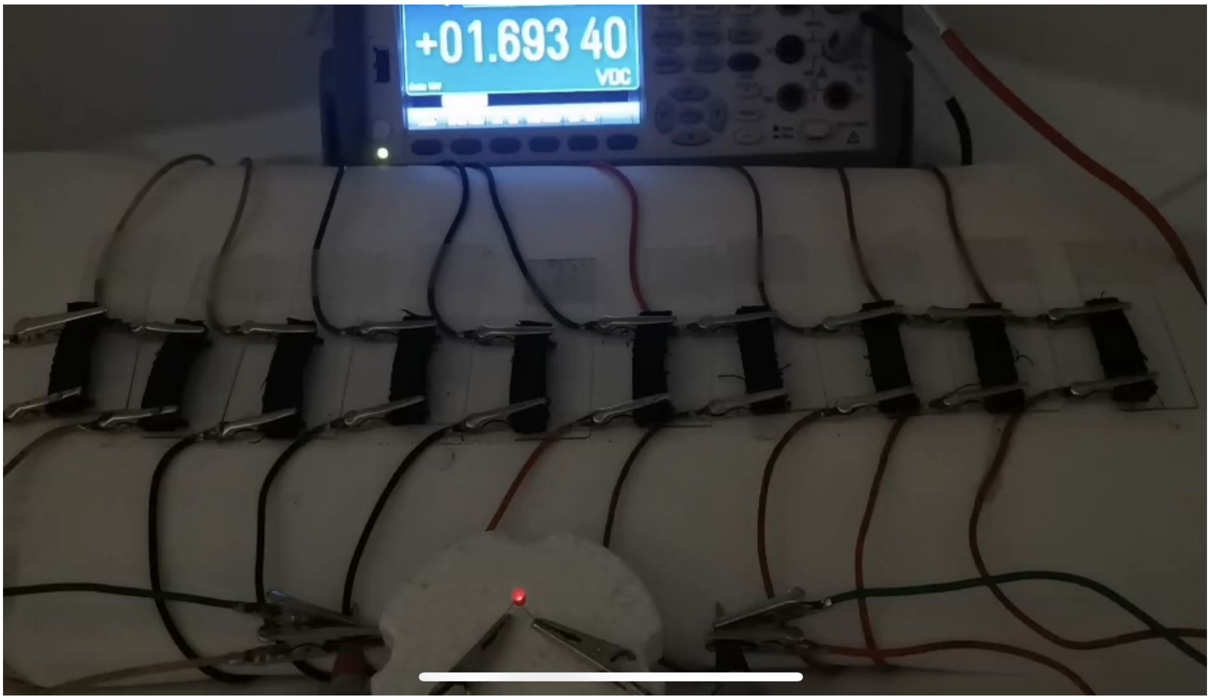

Fig. S1 HENG with a series of 10 × 10 KB6/W used to light up LED. Reprinted with permission from [5], copyright 2023, Elsevier.

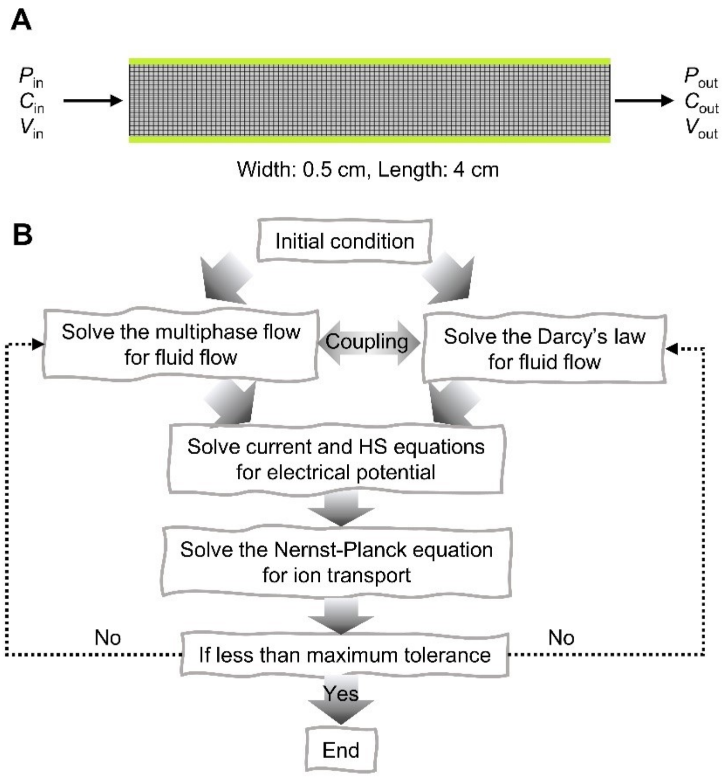

Fig. S2 Numerical simulations of electrical performance of HENGs. (A) Domain of the HENG model. (B) Flow chart for the proposed HENG model. Reprinted (A) with permission from [6], copyright 2024, Cell Press.

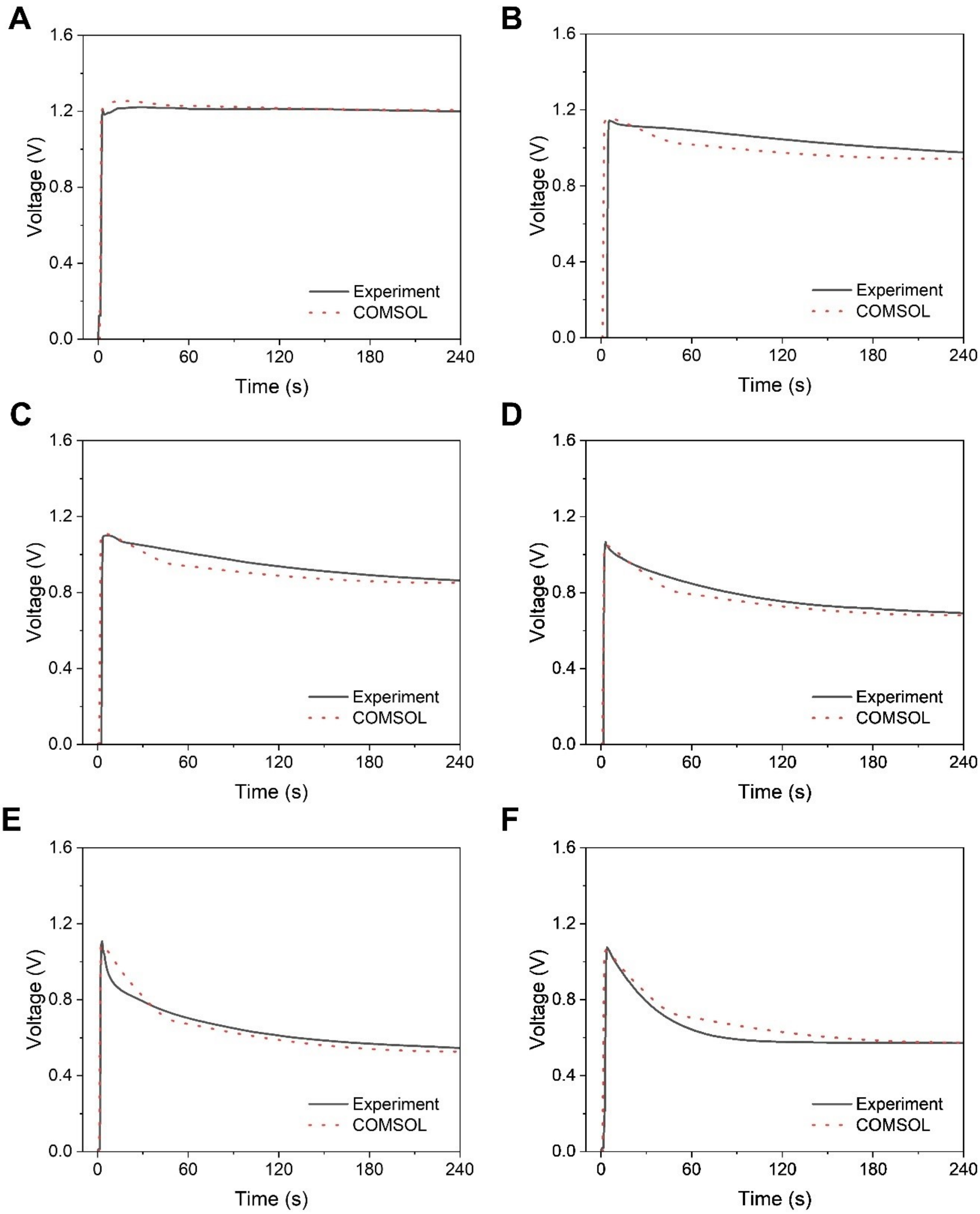

Fig. S3 Experimental and simulated electrical performance of KB-based HENGs with various immersions by 5 M NaCl. (A-F) 1-6 immersions, respectively.

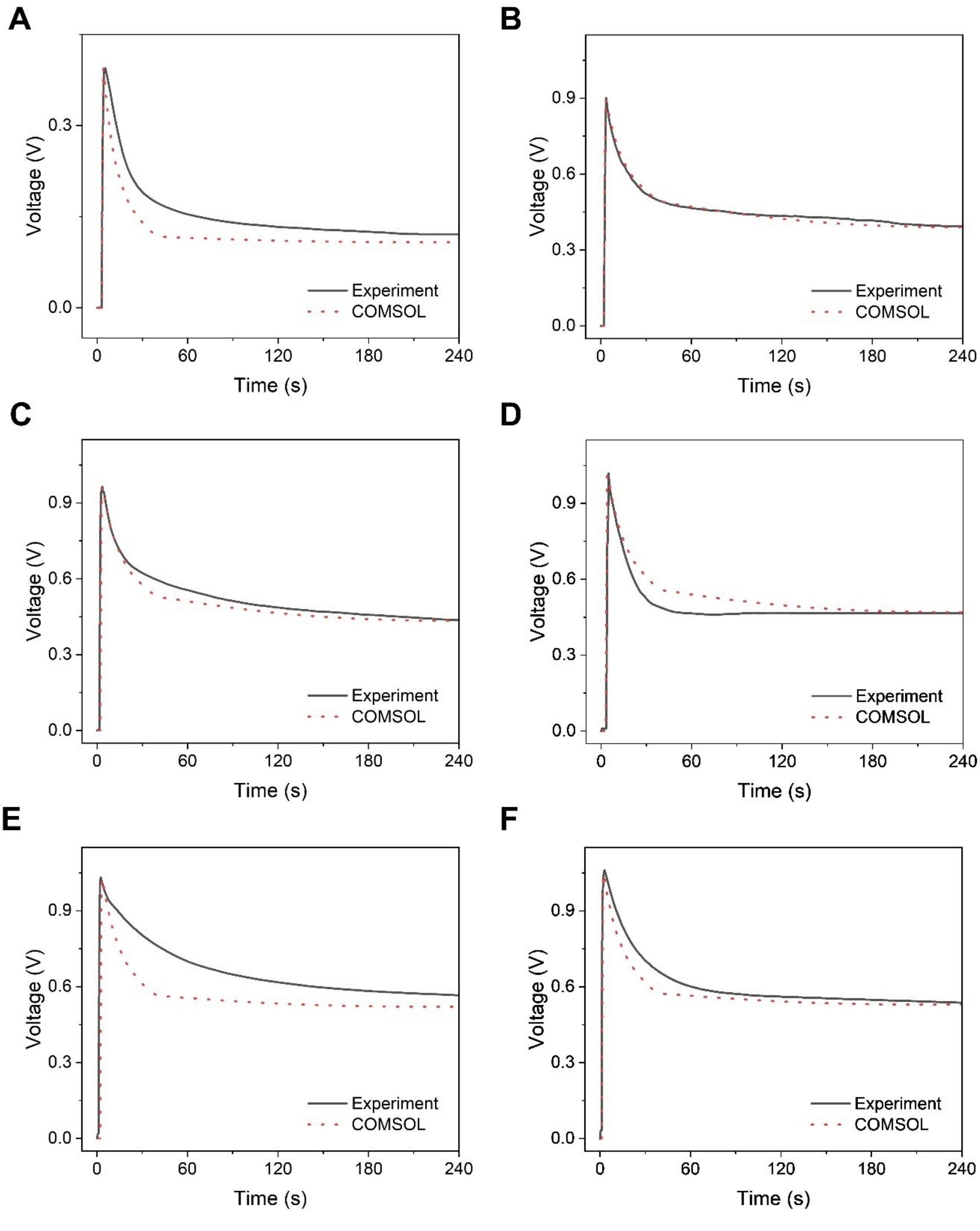

Fig. S4 Experimental and simulated electrical performance of KB6/W-based HENGs with NaCl solutions of various concentrations. (A-F) 0, 0.7, 1.4, 2.1, 2.8, and 3.5 M NaCl, respectively.

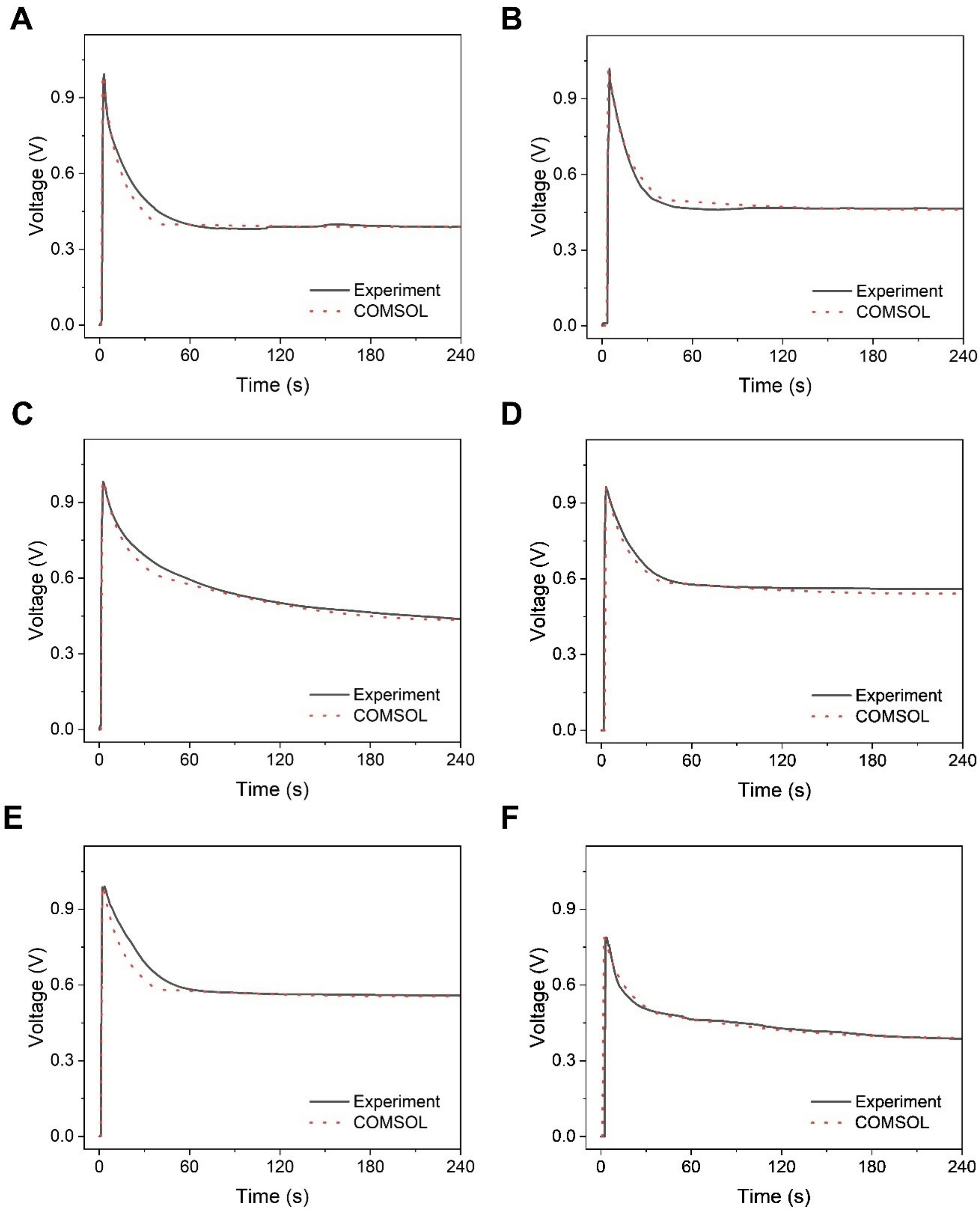

Fig. S5 Experimental and simulated electrical performance of KB6/W-based HENGs with various salts. 2.1 M (A-E) LiCl, NaCl, KCl, $CaCl_2$, and $MgCl_2$, respectively. (F) sweat.

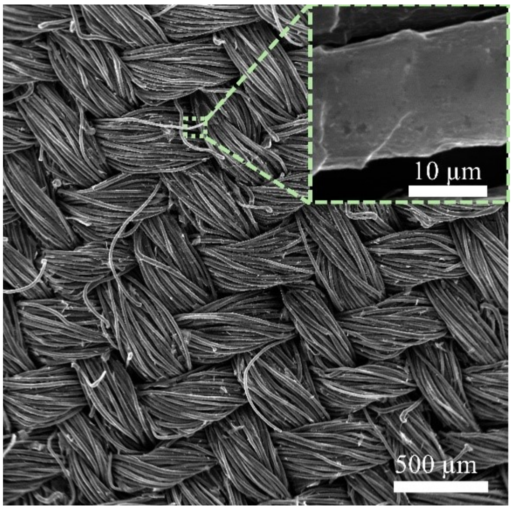

Fig. S6 SEM image of KB@SMX-based HENG.

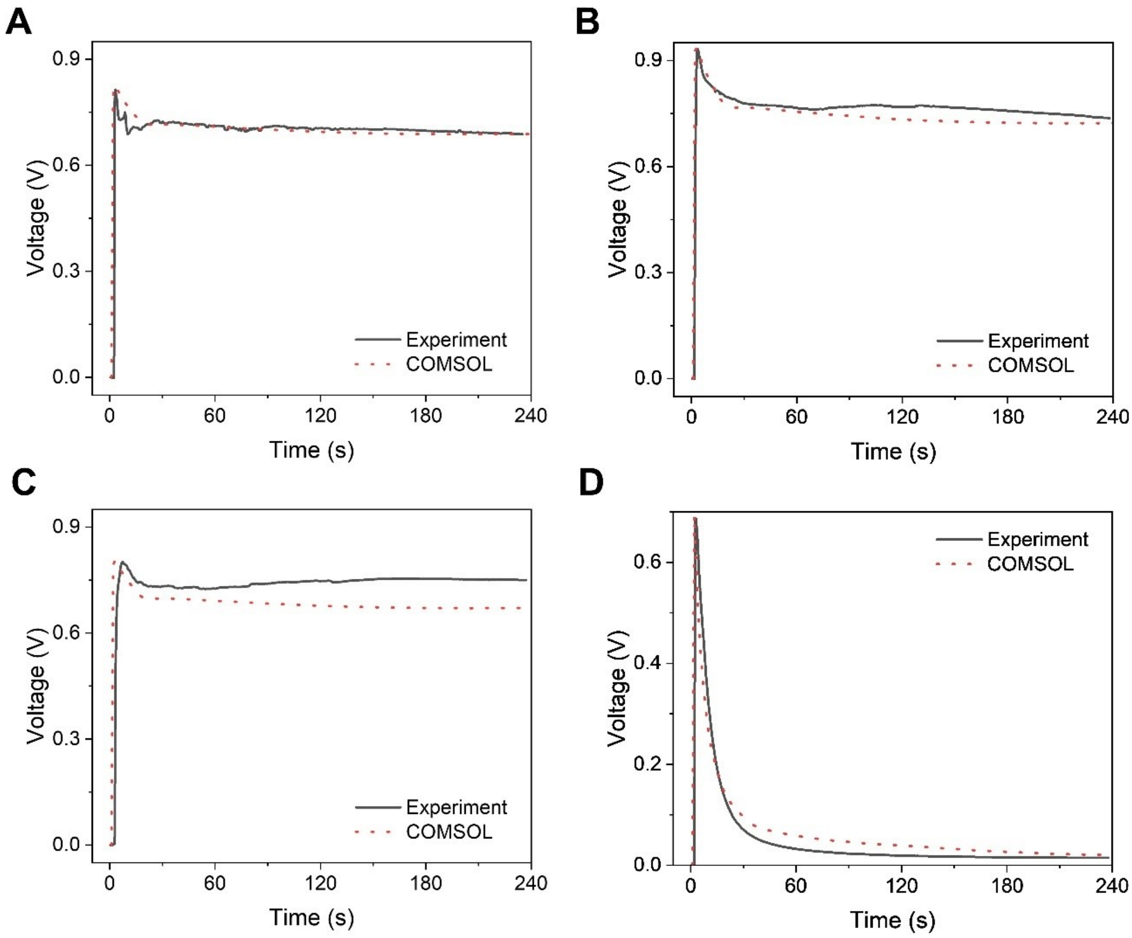

Fig. S7 Experimental and simulated electrical performance of KB@SMX-based HENGs with various ratio of KB:SMX by sweat. KB:SMX ratio of (A) 1:0, (B) 1:1, (C) 1:2, and (D) 0:1, respectively.

References

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