

## Supporting Information

# Finite Element Modeling of MXene/PVDF-Based High-Performance Triboelectric Nanogenerators for Self-Powered Wearable Electronics

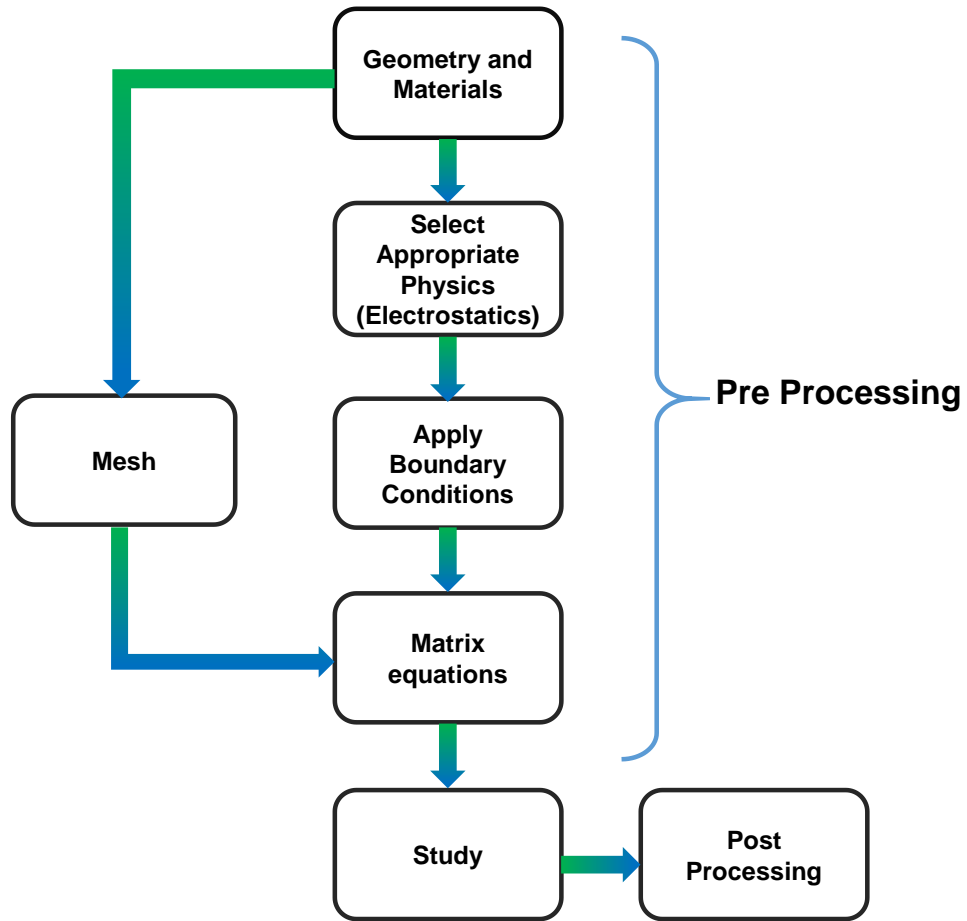
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**Keywords:** Triboelectric nanogenerators, self-powered wearable devices, MXene/PVDF TENG, high-performance TENG, single-electrode TENG, contact-separation TENG

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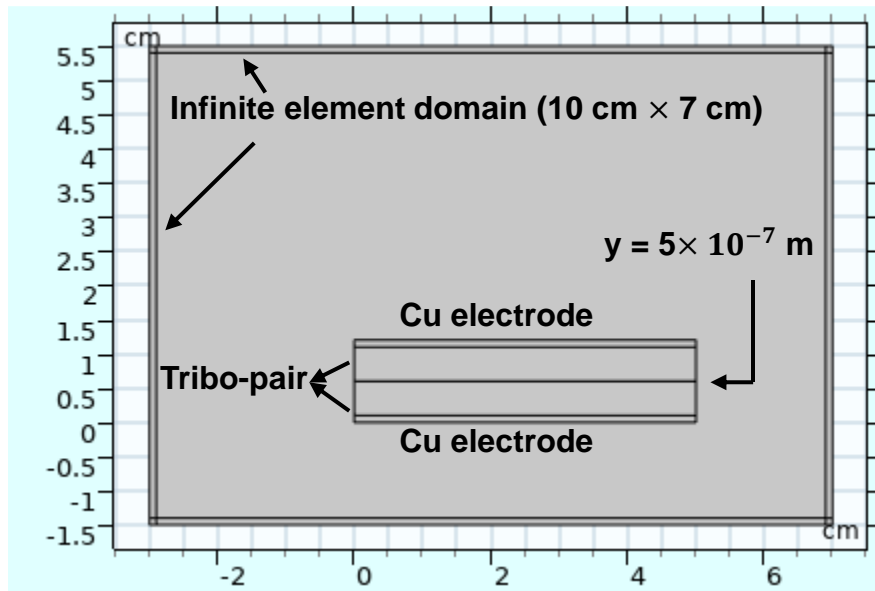
**Workflow of Finite Element Analysis in COMSOL Multiphysics**



**Figure S1.** The finite element analysis workflow in COMSOL Multiphysics.

## Geometry Specification, Boundary Conditions, and Mesh creation

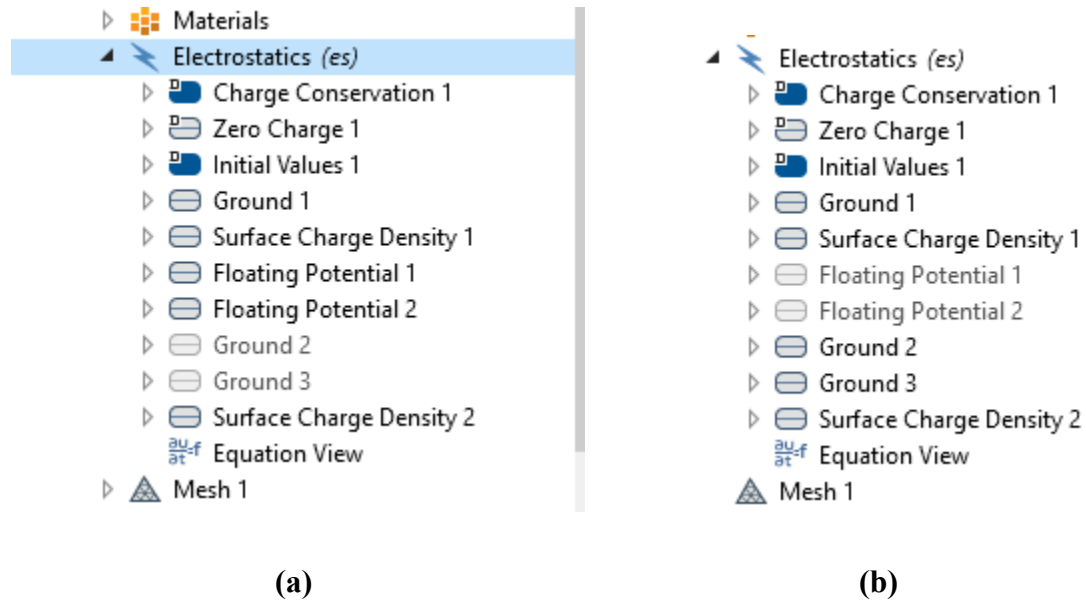
**Model Geometry Specification:** The COMSOL environment generates a 2D geometry of the device. First, a 10 cm by 7 cm square is constructed, significantly larger than the actual device structure. This rectangle represents the infinite element domain required for electrostatic simulation in COMSOL and within which the device geometry was generated. The infinite element domain surrounded the entire shape with 0.2 cm thick layers. These layers were defined as infinite element boundaries. Following the device's specifications, we then developed the device's whole structure. During the creation of structures, only length and height were considered. As the out-of-plane thickness, the device's width was specified. At the time of layer geometry development, a tiny gap was generated between the two tribo-pairs; therefore, selecting the contact surface of each layer to define surface charge density in the physics part became easier. In the parameter section, the value  $y_1 = 5 \times 10^{-7}$  m was specified as the distance between tribo-pairs. This void will be later swept to compute the device's properties.



**Figure S2.** Details of geometry specification of CS-TENG structure in COMSOL.

### Definition of boundary conditions:

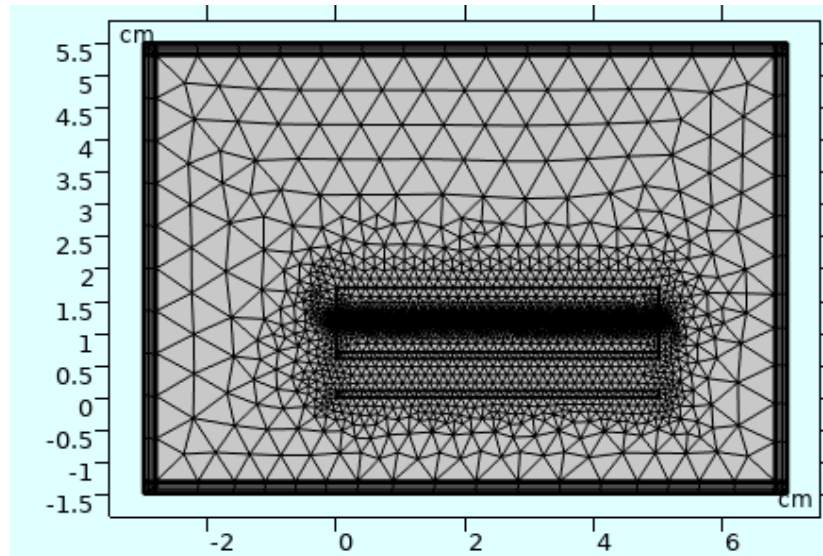
For open-circuit conditions, two floating potentials were defined on the outside surfaces of the contact electrodes, and the charge  $Q$  was set to zero. To calculate the transferred charge under a short-circuit state, the floating potentials had to be turned off, and in their place, two additional ground terminals were defined at the contact electrodes with zero voltage. The out-of-plane thickness was also specified as equal to the geometry's width. Consequently, all boundary criteria were defined.



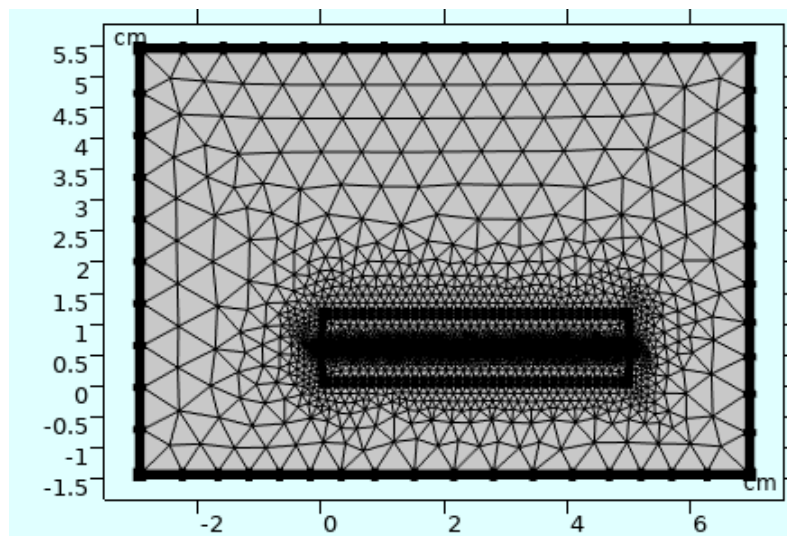
**Figure S3.** Boundary conditions defined in the electrostatic section: (a) for open-circuit condition, and (b) for short-circuit condition.

## Creating Appropriate Mesh

Electrostatics physics-controlled mesh was created. Element size was kept fine.



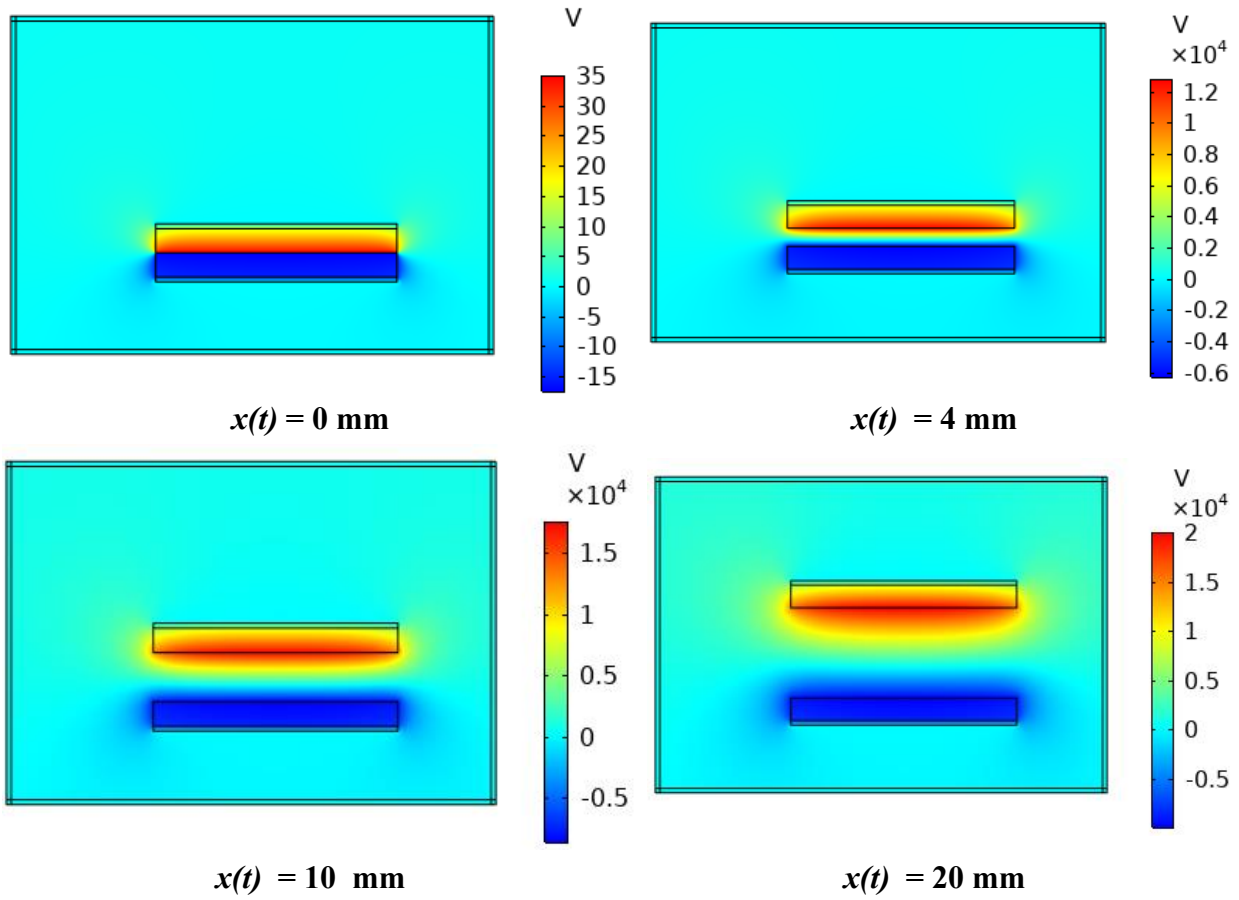
(a)



(b)

**Figure S4.** Physics-controlled mesh generated for the device: (a) SE-TENG, and (b) CS-TENG.

**Potential Distribution of CS-TENG at various separations between tribo-pairs**



**Figure S5.** Potential distribution of CS-TENG at various vertical separation distances between the tribo-pairs.