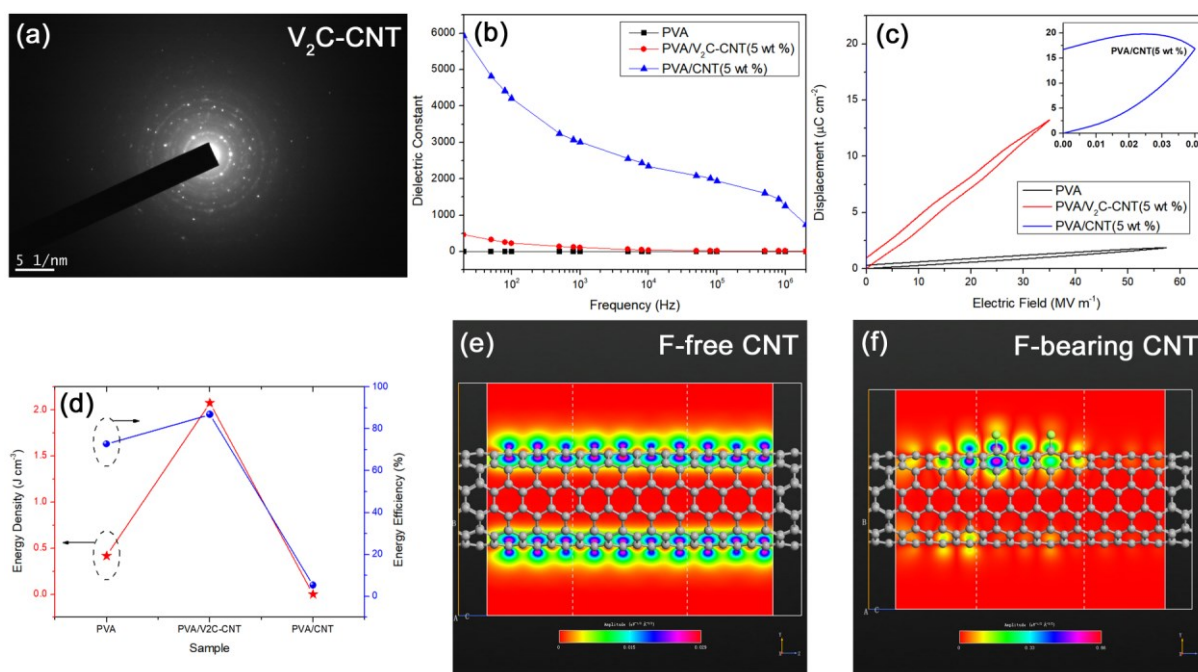


## Supporting Information for Publication

### Interfacial fluorine migration-induced low leakage conduction in PVA based high-*k* composites with V<sub>2</sub>C MXene-SWCNT switchboard-like ceramic *via ab initio* MD simulations

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In Fig. S1a, selection area electron diffraction (SAED) result of hybrid filler was given based on JEM-200CX. In Fig. S1b, dielectric relaxation of composites (two systems with 5 wt % fillers) was found. In Fig. S1c, mono-polar electric hysteresis loops (D-E loops) of composites at 10 Hz were obtained based on ferroelectric analyzer (Premiere II, Radiant). Good loop shape was gained in ternary composite with 5 wt % hybrid filler. Huge leakage conduction based on fat loop was verified in binary composite with 5 wt % CNTs. In Fig. S1d, energy storage traits of two composites with 5 wt % fillers were displayed. Optimal ternary composite could have the improved energy storage properties compared with binary composite and neat polymer. In Figs. S1e and S1f, the calculated electron-transmission spectra of F-free and F-bearing CNTs were shown based on GGA-PBE of RPBE algorithm, respectively. By comparison, the results here were in high accordance with results in Figs. 11e and 11f. Related conclusions in main text were further confirmed.



**Figure S1.** (a) SAED of hybrid filler, (b) dielectric relaxation of composites, (c) D-E loops of composites, (d) energy storage traits of composites, (e) electron-transmission spectra of F-free CNTs based on GGA-PBE of RPBE algorithm and (f) electron-transmission spectra of F-bearing CNTs based on GGA-PBE of RPBE algorithm.