

Supporting Information

©XMU and CCS

Engineering Small-Sized Cations with Strong Solvation for High-Voltage Supercapacitors

Tong Huo, Pan Liu, Hao Chen, Peng Zhang, Zhen-Lei Chen, Guo-Fu Sun, Zhi-Qiang Shi*, Jing Wang

College of Materials Science and Engineering, Tianjin Key Laboratory of Advanced Fibers and Energy Storage, Tiangong University, Tianjin 300387, China

*Corresponding e-mails: shizhiqiang@tiangong.edu.cn

Table S1. Composition of simulation systems for various electrolytes in bulk state.

System	# TMA-FSI	# TEA-FSI	# TPA-FSI	#PC
TMF	50	0	0	590
TEF	0	50	0	590
TPF	0	0	50	590

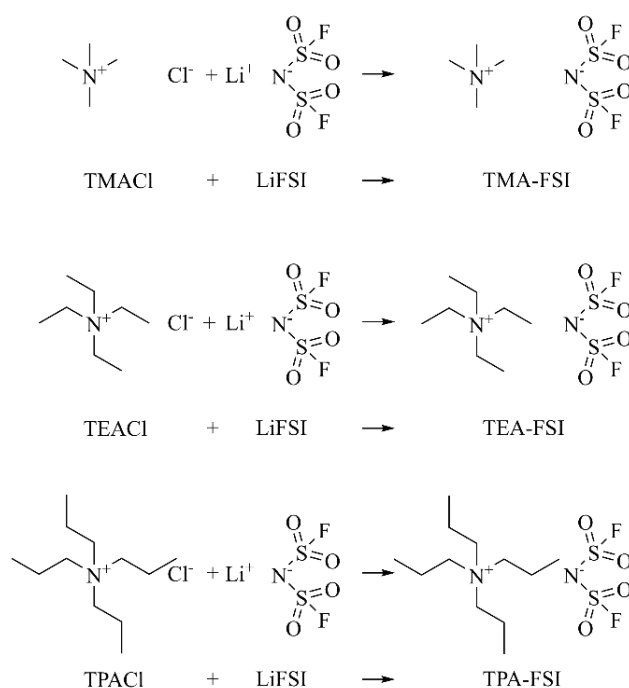


Figure S1. Synthetic route of electrolyte salt (a) TMA-FSI (b) TEA-FSI (c) TPA-FSI.

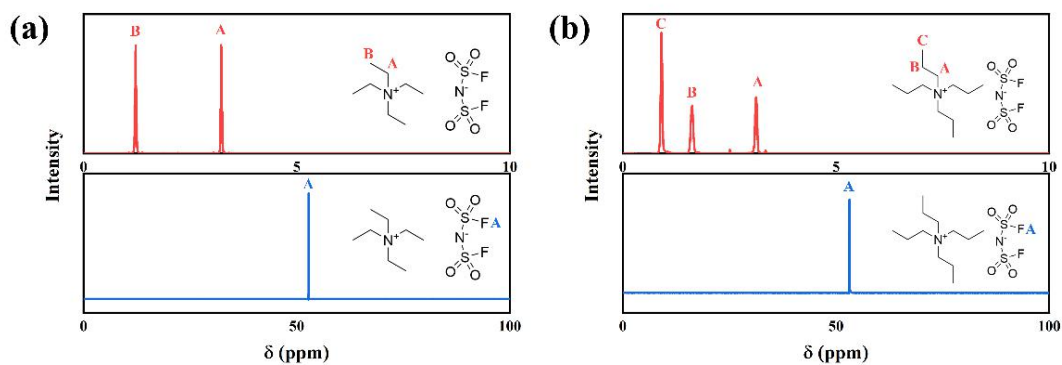


Figure S2. ^1H NMR spectra and ^{19}F NMR spectra of (a) TEA-FSI and (b) TPA-FSI electrolyte

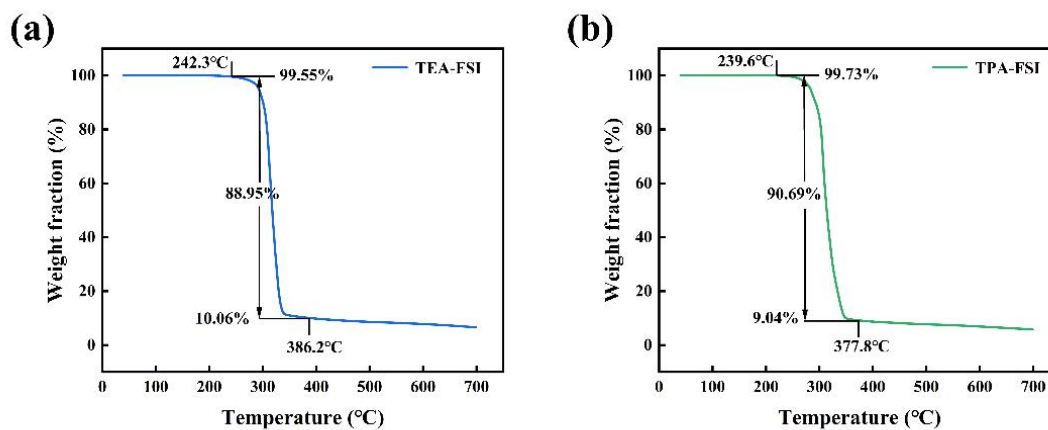


Figure S3. Thermogravimetric curve of (a) TEA-FSI and (b) TPA-FSI electrolyte.



Figure S4. Physical appearance of TMA-FSI, TEA-FSI, TPA-FSI, TMF, TEF and TPF.

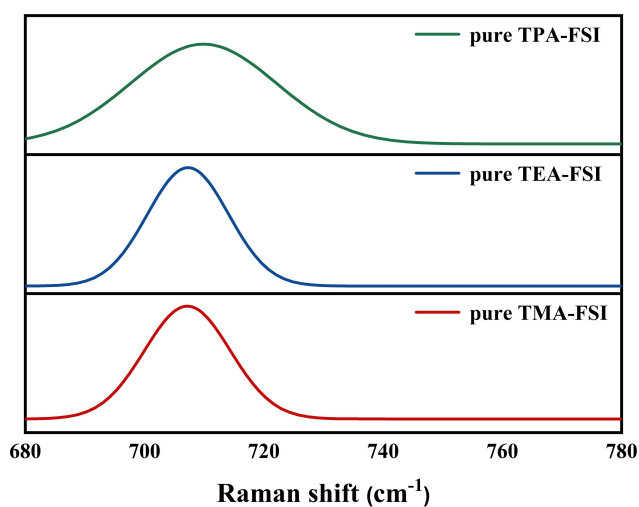


Figure S5. Raman spectra of the characteristic peaks of FSI⁻

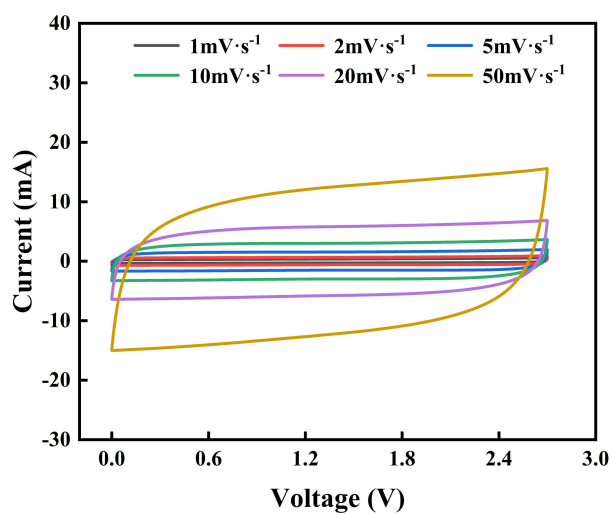


Figure S6. CV curves at different scan rates of the 2.7 V.

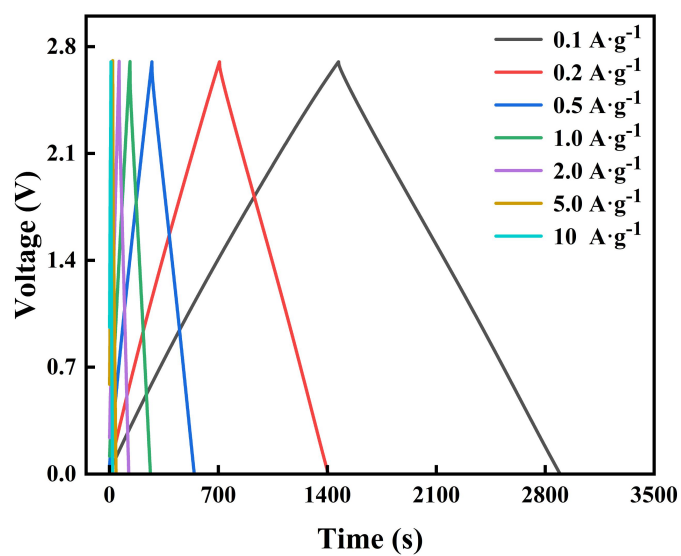


Figure S7. GCD curves at different current densities of the 2.7 V.

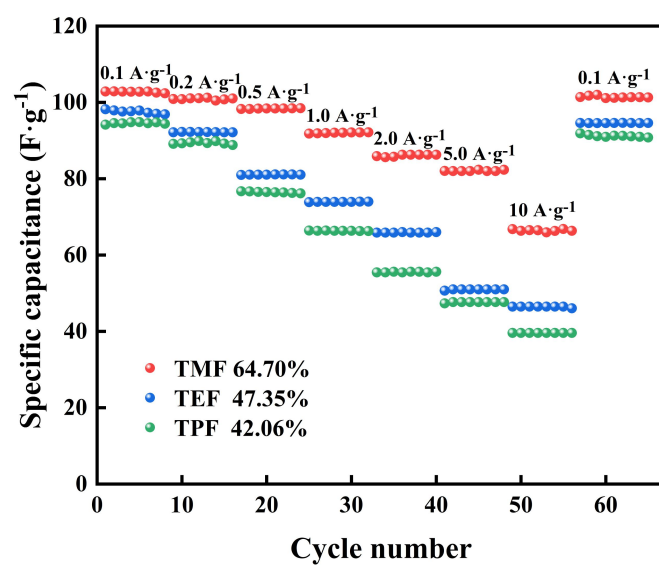


Figure S8. Specific capacitance at different current densities of the 2.7 V.

Statements & Declarations

Acknowledgements

This work was supported by the National Natural Science Foundation of China (No.22179094 and No.52407249), the Natural Science Foundation of Tianjin (No.23JCQNJC00880), and the Hebei Provincial Doctoral Innovation Workstation (No.195). The authors also would like to express their gratitude to the Analytical Testing Center of Tiangong University for the technical support and material characterization.

Conflicts of Interest

Authors declare no conflict of interest.

Data Availability

All data are available in the main text or the supplementary materials.

Author Contributions

Tong Huo, Pan Liu, Hao Chen, Peng Zhang, Zhen-Lei Chen, Guo-Fu Sun, Zhi-Qiang Shi, Jing Wang jointly conceived the work. Tong Huo and Guo-Fu Sun performed material synthesis and characterisation. Pan Liu, Peng Zhang and Zhen-Lei Chen conducted the MD and DFT calculations. Hao Chen collected and analysed the NMR and Raman spectra. Tong Huo, Zhi-Qiang Shi and Jing Wang jointly drafted the manuscript. All authors discussed the experimental content and the final manuscript.

Ethics Approval

Authors declare that no human or animal subjects were involved in this study, and no ethical approval was required.

Consent to Participate

Authors declare that no human subjects were involved in this study.

Consent to Publish

Publication consent has been obtained from all participants.