Supplementary Information

Wide Electrochemical Window Ionic Salt for use in Electropositive Metal Electrodeposition and Solid State Li-ion Batteries

Sankaran Murugesan^a, Oliver A. Quintero^a, Brendan P. Chou^a, Penghao Xiao^a, Kyusung Park^b, Justin W. Hall^a, Richard A. Jones^a, Graeme Henkelman^a, John B. Goodenough^b and Keith J. Stevenson^{a*}

^aDepartment of Chemistry and Biochemistry, The University of Texas at Austin, 1 University Station, Austin, Texas, 78712, USA

^bTexas Materials Institute and Materials Science and Engineering Program, The University of

Texas at Austin, Austin, Texas 78712, United States

^{*} Corresponding author: Keith J. Stevenson (stevenson@mail.cm.utexas.edu) (T) +1-512- 232- 9160; (F) +1-512-471-8696



Figure S1a. ¹H NMR spectrum of PP₁₃PF₆ in CD₂Cl₂.



Figure S1b. ¹³C NMR spectrum of PP₁₃PF₆ in CD₂Cl₂.



Figure S1c. ¹⁹F NMR spectrum of PP₁₃PF₆ in CD₂Cl₂.



Figure S1d. ³¹P NMR spectrum of PP₁₃PF₆ in CD₂Cl₂.



Figure S1e. FTIR (diamond ATR) spectrum of PP₁₃PF₆.



Figure S1f. Positive ion mass spectrum of PP₁₃PF₆.



Figure S1g. Negative ion mass spectrum of PP₁₃PF₆.



Figure S2. XRD of electrodeposited Sn over stainless steel electrode (red line) and blue lines shows the standard Sn (JCPDS#65-2631).



Figure S3. Experimental powder XRD of $PP_{13}PF_6$ (red line) compared with the theoretically generated XRD pattern (blue line) using the single crystal structure.



Figure S4. Calculated electrostatic potential of Li showing the lithium vacuum level at 2.33 eV. The Fermi-level is calculated as -0.67 eV.



Figure S5. Calculated electrostatic potential of $PP_{13}PF_6$, showing a vacuum level of 2.39 eV and a Fermi-level of -6.20 eV.



Figure S6. Cyclic voltammograms of $PP_{13}PF_6$ using the asymmetric cell (Li metal/ $PP_{13}PF_6$ + 10wt% LiTFSI)/stainless steel block) with different temperatures at the scan rate of 2 mV/s.

| Symmetric cell | | | | | | |
|-----------------|-------------|----------------|----------------|------------------------------------|---------------------------|---------|
| Temp (°C) | Temp (K) | (1/K) | R _p | $Conductivity\left(\sigma\right)$ | $\log\left(\sigma\right)$ | ln (o) |
| 22.7 | 295.7 | 0.00338 | 76718 | 2.06E-06 | -5.6852 | -13.091 |
| 32 | 305 | 0.00328 | 33994 | 4.66E-06 | -5.3317 | -12.277 |
| 35 | 308 | 0.00325 | 24387 | 6.49E-06 | -5.18746 | -11.945 |
| 40 | 313 | 0.00320 | 5059 | 3.13E-05 | -4.50436 | -10.372 |
| 45 | 318 | 0.00315 | 2158 | 7.34E-05 | -4.13435 | -9.520 |
| Asymmetric cell | | | | | | |
| 25 | 298 | 0.00335 | 1.08E+05 | 3.78E-07 | -6.42296 | -14.789 |
| 30 | 303 | 0.00330 | 1.66E+04 | 9.31E-06 | -5.03105 | -11.584 |
| 35 | 308 | 0.00325 | 9.64E+03 | 1.61E-05 | -4.79401 | -11.039 |
| 40 | 313 | 0.00320 | 2.24E+03 | 6.90E-05 | -4.16118 | -9.581 |
| 45 | 318 | 0.00314 | 6.48E+02 | 2.39E-04 | -3.62166 | -8.339 |

 Table S1. Impedance and conductivity data of symmetric and asymmetric cells.