Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.
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Electronic Supplementary Information for

A Symmetric Organic - Based Nonaqueous Redox Flow Battery and Its State of Charge Diagnostics by FTIR

Wentao Duan,†[a,b] Rama S. Vemuri,†[a,b] Jarrod D. Milshtein,[a,c] Sydney Laramie,[a,d] Rylan D. Dmello,[a,e] Jinhua Huang,[a,f] Lu Zhang,[a,f] Dehong Hu,[b] M. Vijayakumar,[a,b] Wei Wang,[a,b] Jun Liu,[a,b] Robert M. Darling,[a,g] Levi Thompson,[a,d] Kyle Smith,[a,e] Jeffery S. Moore,[a,e] Fikile R. Brushett*[a,c] and Xiaoliang Wei*[a,b]

[a] Joint Center for Energy Storage Research (JCESR)

[b] Pacific Northwest National Laboratory, 902 Battelle Blvd, Richland, WA 99352, USA

[c] Massachusetts Institute of Technology, 77 Massachusetts Ave, Cambridge, MA 02139, USA

[d] University of Michigan, 500 S State St, Ann Arbor, MI 48109, USA

[e] University of Illinois Urbana-Champaign, 405 North Mathews Ave, Urbana, IL 61801, USA

[f] Argonne National Laboratory, 9700 South Cass Ave, Argonne, IL 60439, USA

[g] United Technologies Research Center, 411 Silver Lane, East Hartford, CT 06108, USA

† These authors contributed equally to this work.

***Corresponding authors**:

X. Wei: Email: Xiaoliang.Wei@pnnl.gov.

F. R. Brushett: Email: brushett@mit.edu.

Supporting Figures

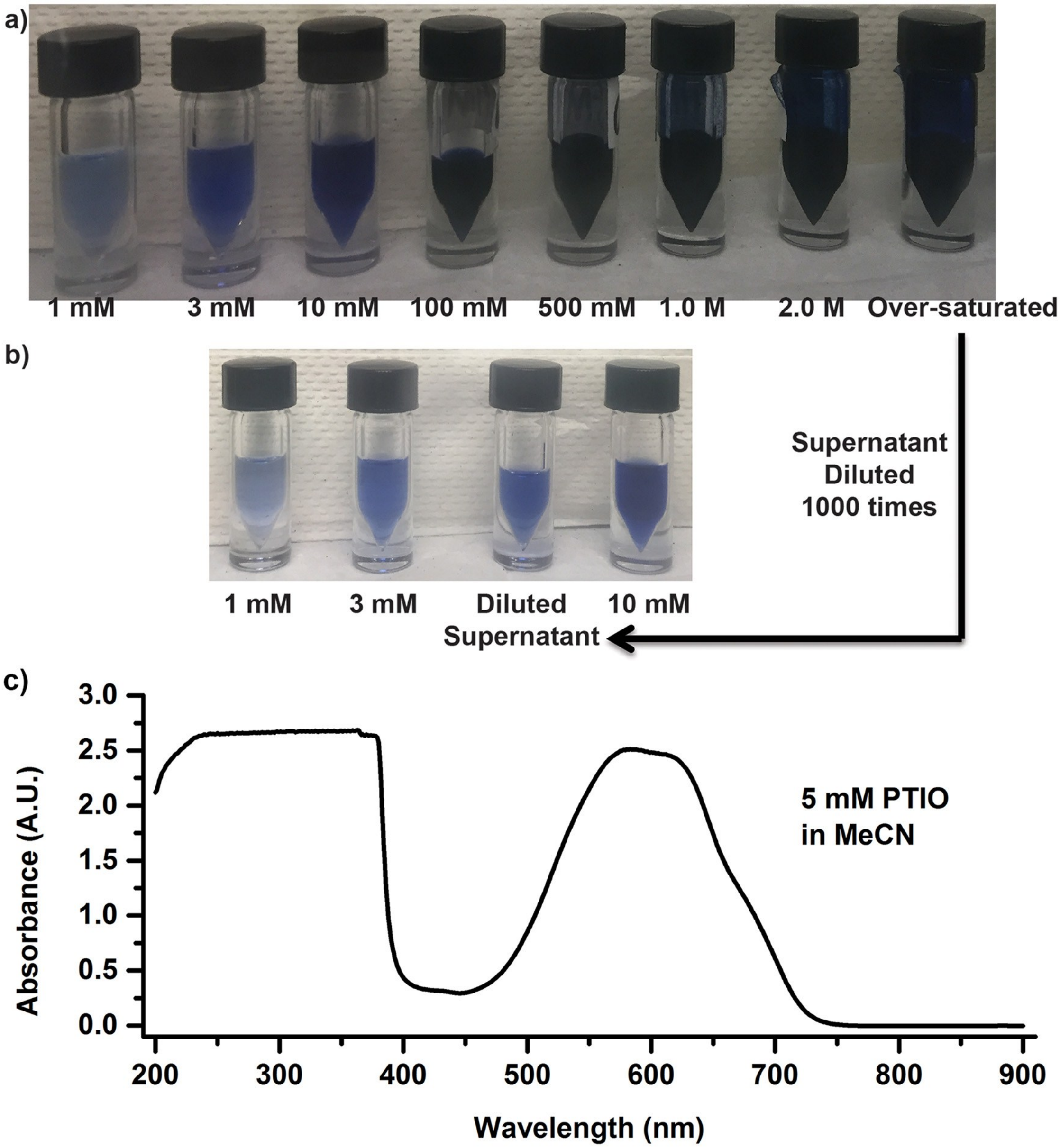

Figure S1. PTIO solubility measurements in MeCN: (a) photographs of a series of PTIO solutions in MeCN at different concentrations of 1 mM, 3 mM, 10 mM, 100 mM, 500 mM, 1.0 M, 2.0 M, and oversaturated; (b) photographic comparison of the 1000-fold diluted supernatant from the oversaturated PTIO solution with other PTIO solutions, with the former closest to the 3mM one; (c) the UV-vis spectrum of the 5 mM PTIO solution in MeCN showing that PTIO has strong absorption, which explains the similarly deep-blue solution color at ≥0.1 M PTIO.

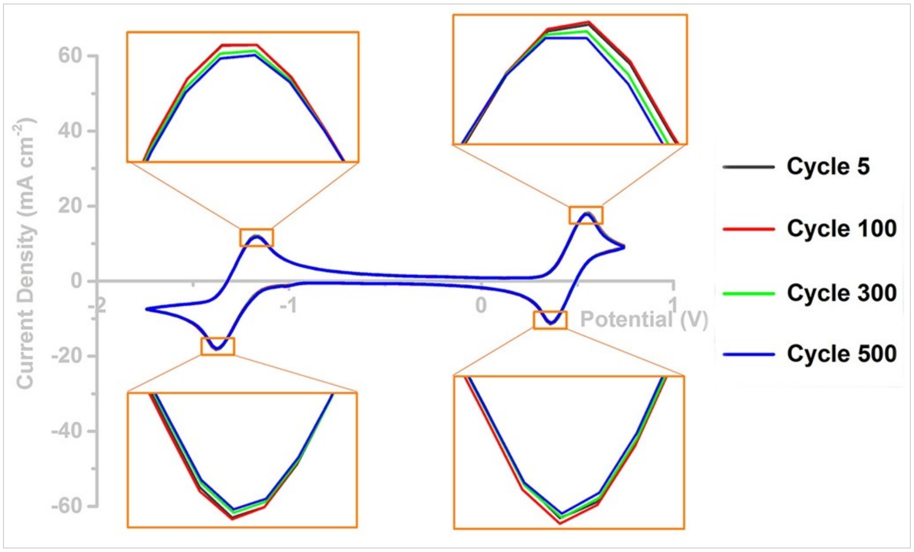

Figure S2. Expanded view of the redox peaks in the repeated CV scans of PTIO (Figure 1a), showing respective CV curves of the 5th, 100th, 300th and 500th cycles.

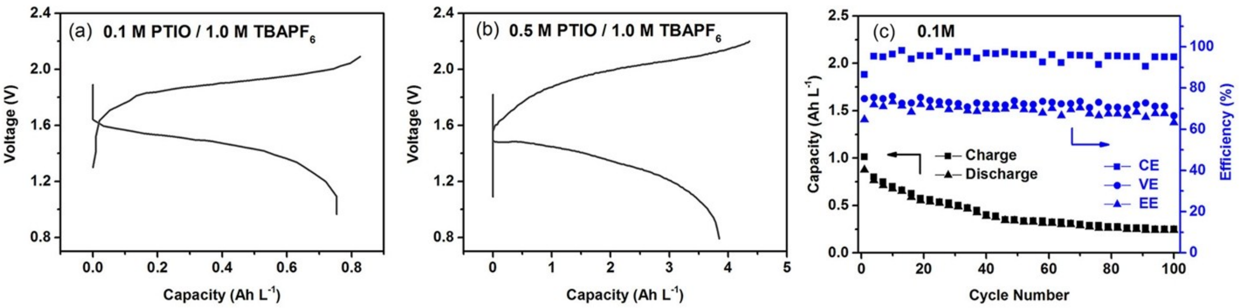

Figure S3. The voltage curves of the PTIO flow cells using (a) 0.1 M PTIO; and (b) 0.5 M PTIO; (c) cycling efficiency and capacity of the 0.1 M PTIO flow cell for 100 cycles. The supporting electrolyte was 1.0 M TBAPF$_6$ in MeCN. The current density was 20 mA cm^{-2}.

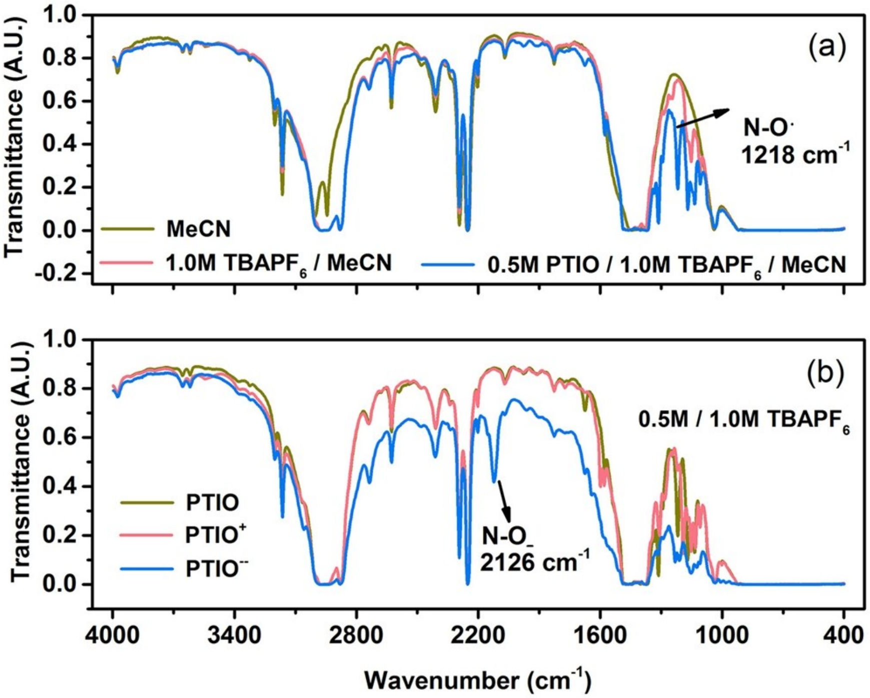

Figure S4. Full range FTIR spectra of the PTIO electrolyte systems: (a) MeCN, 1.0 M $TBAPF_6$/MeCN, and 0.5 M PTIO in 1.0 M $TBAPF_6$/MeCN; (b) 0.5 M PTIO and charge species ($PTIO^+$ and $PTIO^-$) in 1.0 M $TBAPF_6$/MeCN.

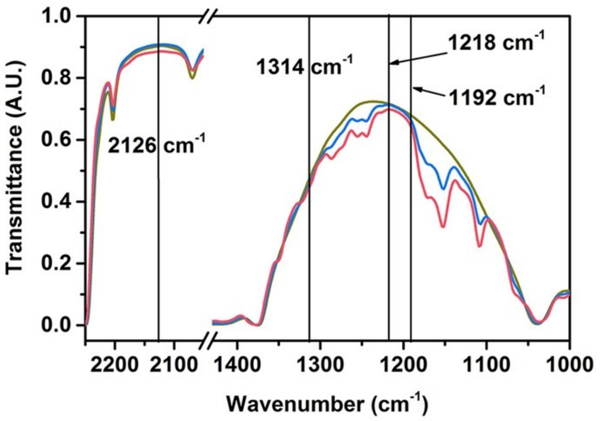

Figure S5. The FTIR spectra of the $TBAPF_6$ salt (charge carrier) at 0, 0.5 M, and 1.0 M concentrations in the range of 1400-1000 cm^{-1}. Dark yellow: MeCN; Blue: 0.5 M $TBAPF_6$/MeCN; Red: 1.0 M $TBAPF_6$/MeCN.

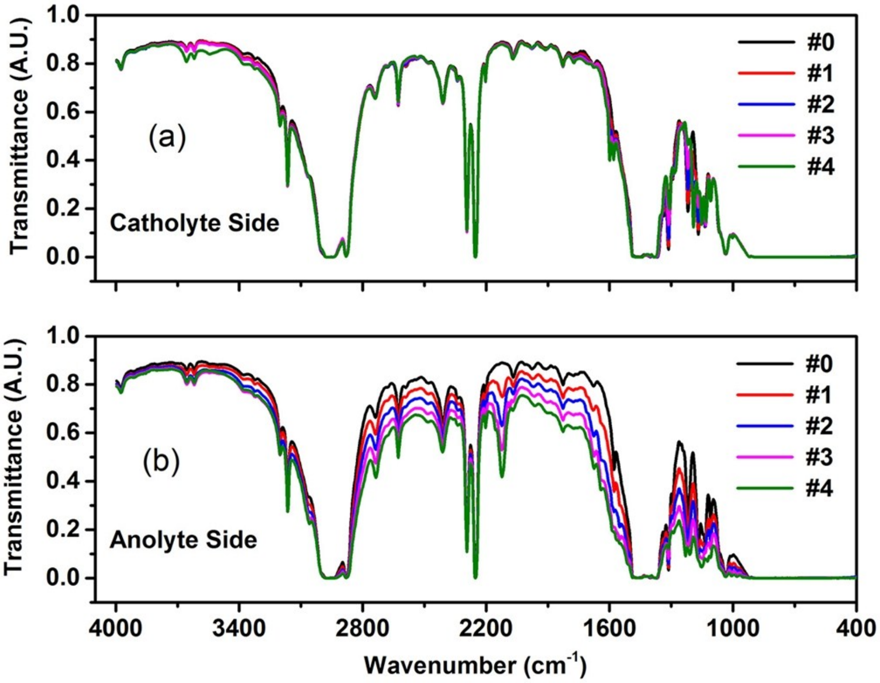

Figure S6. The FTIR spectra of the samples #0-4: (a) from the catholyte side; and (b) from the anolyte side.

Scheme S1. Derivation of the linear relationship between the transmittance (T) and [PTIO].

The real transmittance (T_{real}) and the concentration ([PTIO]) of PTIO satisfy the Beer-Lambert Law (Equation S1):

$$-log(T_{real}) = \varepsilon b[PTIO] \tag{S1}$$

where ε is the absorptivity coefficient and b is the path length. Because the supporting electrolyte of 1.0 M $TBAPF_6$/MeCN is the spectral background, the T_{real} of PTIO can be calculated by the nominal transmittance (T) divided by the electrolyte background transmittance (T_0) in the FTIR spectra (Equation S2).

$$T_{real} = \frac{T}{T_0} \tag{S2}$$

Thus, from Equations S1 and S2, we can derive Equation 1 in the main text:

$$-log(T) = \varepsilon b[PTIO] - log(T_0) \tag{1}$$