Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for:

Na Intercalation in Fe-MIL-100 for Aqueous Na-ion Batteries

James S. Chavez, Katharine L. Harrison, and Dorina F. Sava Gallis*

Nanoscale Sciences Department, Sandia National Laboratories, Albuquerque, NM 87185, USA.

Figure S1. Cyclic voltammograms of a molarity study performed on micro-Fe-MIL-100 with Nafion at 0.1mV/s. Data shown is of the first cycle.

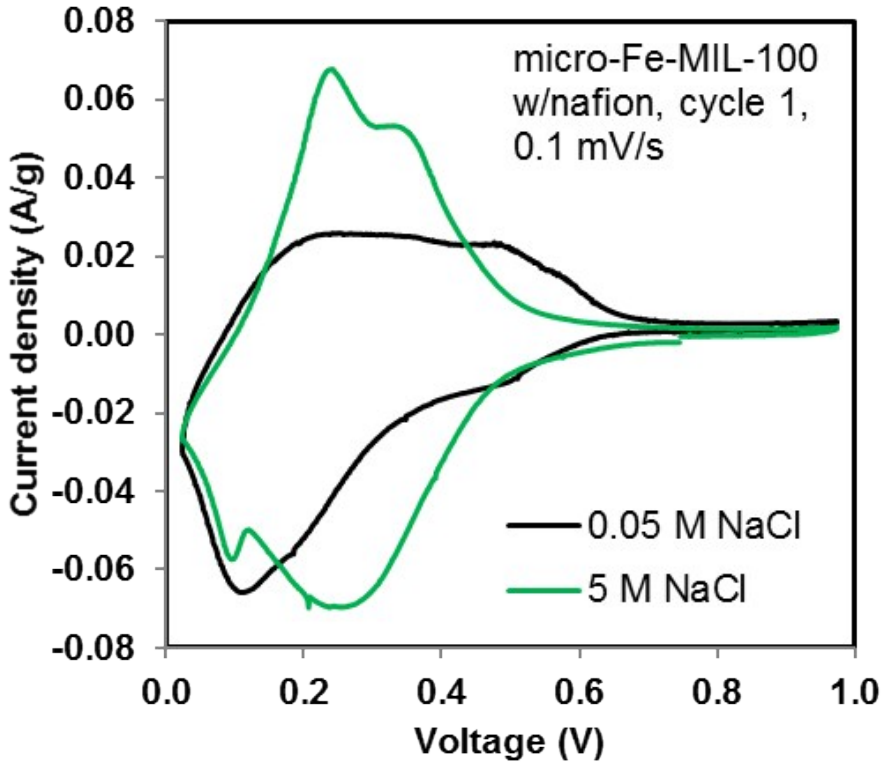


Figure S2. Galvanostatic sodiation of pristine Fe-MIL-100 (Nafion binder) against a Pt counter electrode versus an Ag/AgCl reference electrode ("Cycle 1 CE sodiation") which was later used as a counter electrode and galvanostatic sodiation of pristine Fe-MIL-100 (Nafion binder) against the presodiated Fe-MIL-100 counter electrode versus an Ag/AgCl reference electrode ("Cycle 1 WE"). Voltage is presented versus SHE. Note that the rate was faster for the CE sodiation and the electrode was much thicker, giving rise to larger overpotential. The cutoff voltage was higher for the CE sodiation to avoid the bubble formation that occurred at the Pt counter electrode.

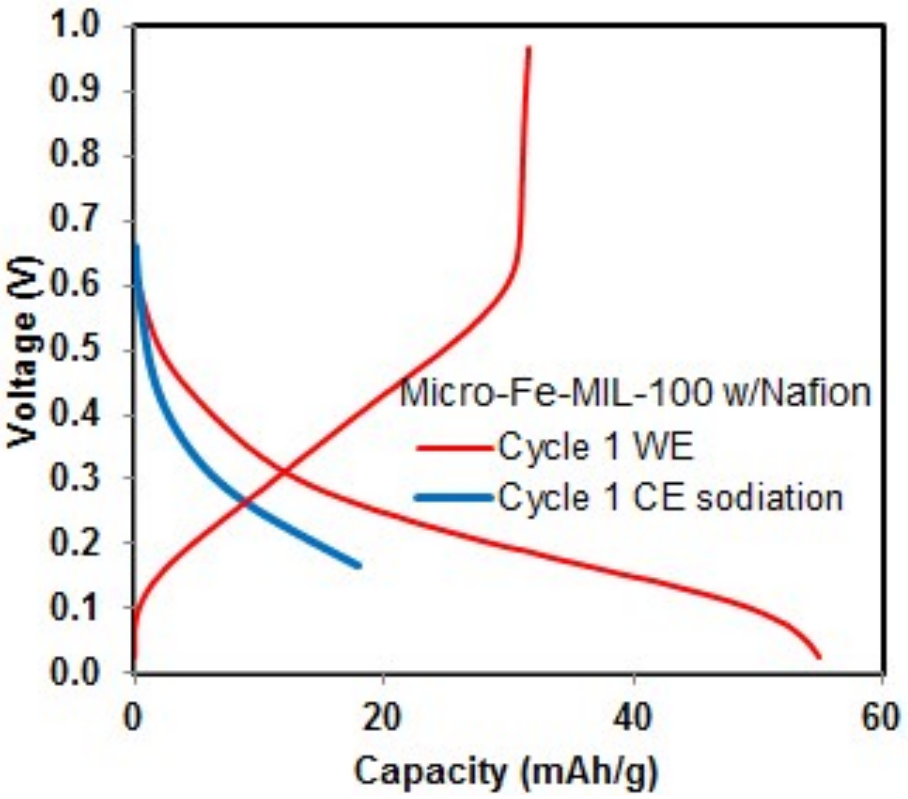


Figure S3. Voltage profiles versus Na^+/Na during the 1st cycle in organic vs aqueous electrolytes.

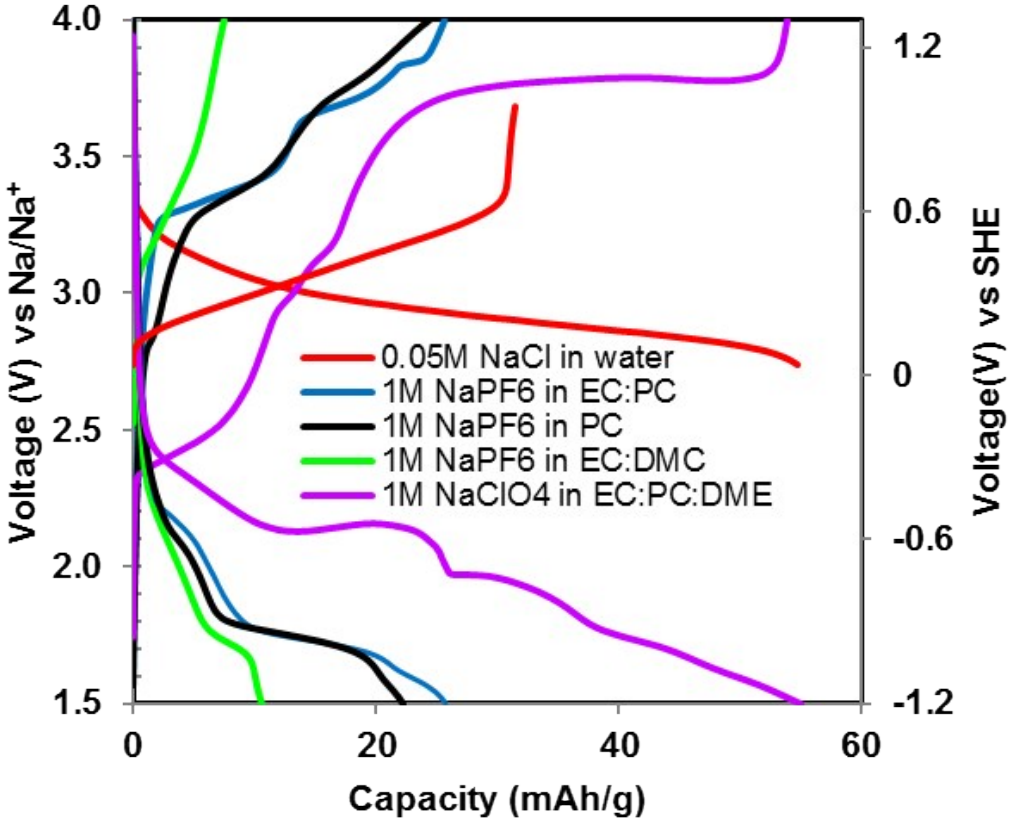


Figure S4. Powder X-ray diffraction of pristine nano-Fe-MIL-100 (orange), as-made electrode (fuchsia) and cycled electrodes with various compositions: Kynar (black), Nafion® (red), and no binder (green). Cycled electrodes were characterized in their desodiated state after 30 galvanostatic cycles in 0.05M NaCl at C/3. The lack of sharp peaks is related to the nanostructure nature of the sample and is comparable with powder X-ray diffraction data from previous reports of nano-Fe-MIL-100.[1]

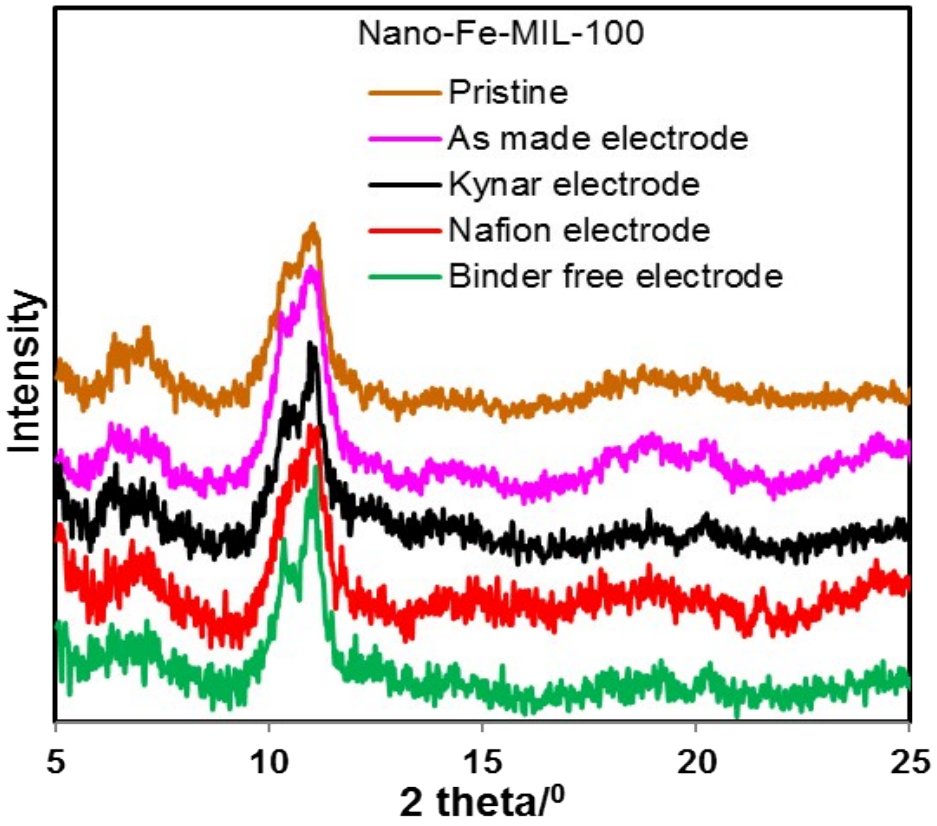


Figure S5. Voltage vs. capacity graphs (left) and differential capacity analysis (right) for various compositions of Nano-Fe-MIL-100: (a,b) Kynar, (c,d) Nafion and (e,f) Binder-free electrodes after the 1st, 2nd, 5th and 30th cycles. All cells were cycled at C/3 in 0.05 M NaCl/water electrolyte.

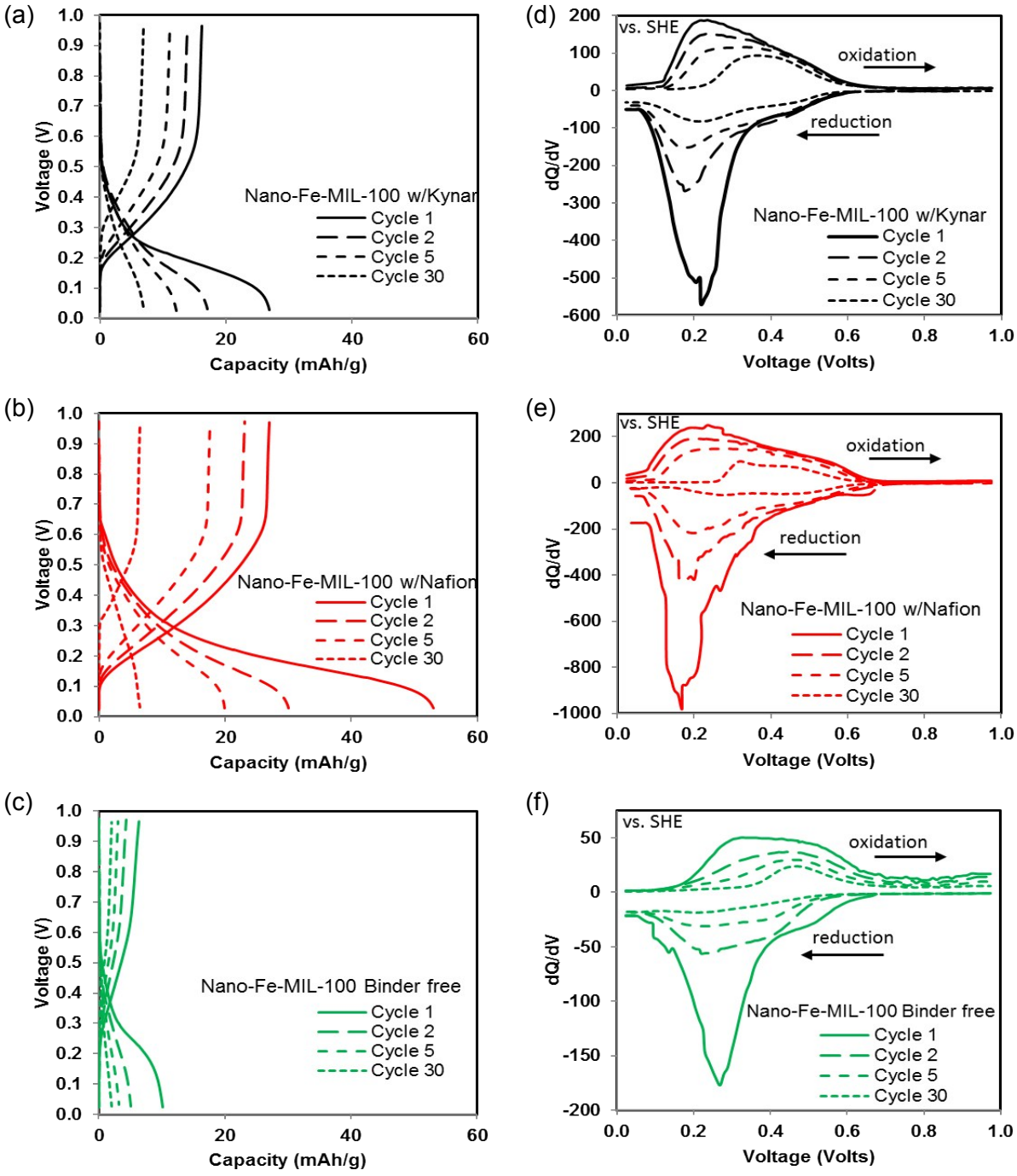


Figure S6. Oxidation peak current plotted against varying scan rates (0.1, 0.25, 0.5, 1, and 2 mV/s) in 0.05 M NaCl/water for micro-Fe-MIL-100 with Nafion binder. The square root dependence of peak potential on scan rate is shown in blue.

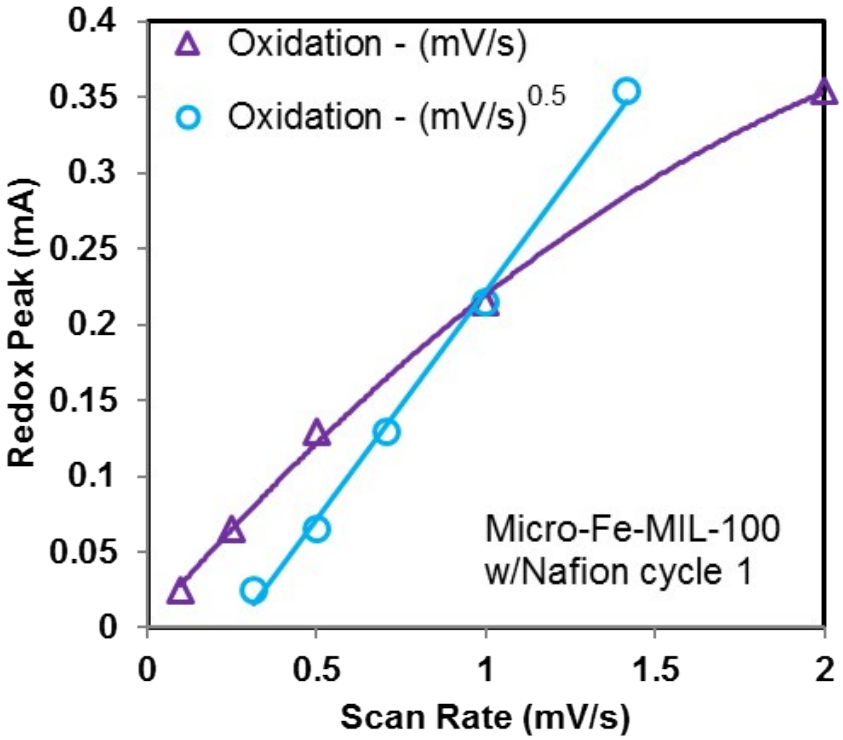
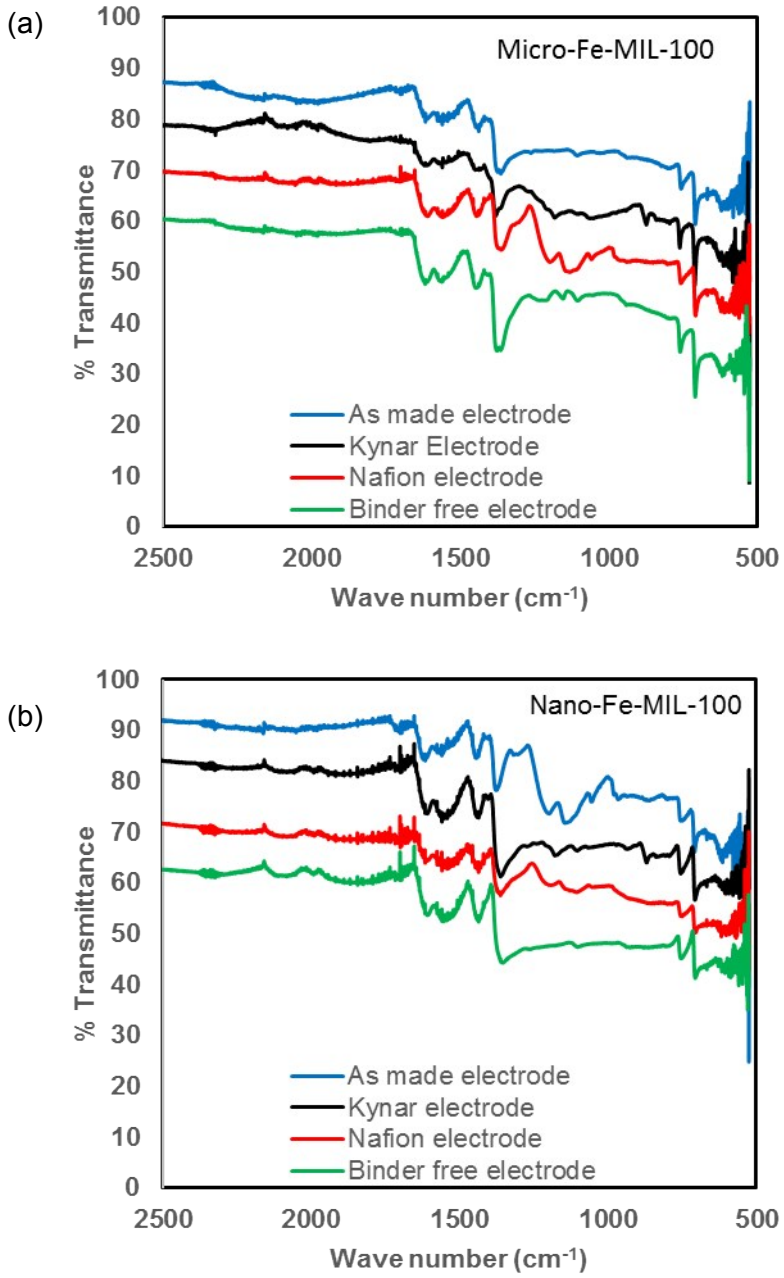


Figure S7. IR spectra for as made (blue) and cycled electrodes with various compositions: Kynar (black), Nafion® (red), and no binder (green) for (a) Micro-Fe-MIL-100 samples, and (b) Nano-Fe-MIL-100 samples. Cycled electrodes were characterized in their desodiated state after 30 galvanostatic cycles in 0.05M NaCl at C/3.



References:

1. A. García Márquez, A. Demessence, A. E. Platero-Prats, D. Heurtaux, P. Horcajada, C. Serre, J.-S. Chang, G. Férey, V. A. de la Peña-O'Shea, C. Boissière, D. Grosso and C. Sanchez, *Eur. J. Inorg. Chem.*, 2012, **32**, 5165-5174.