

# Correction to “A Dual-Ion Battery Cathode via Oxidative Insertion of Anions in a Metal–Organic Framework”

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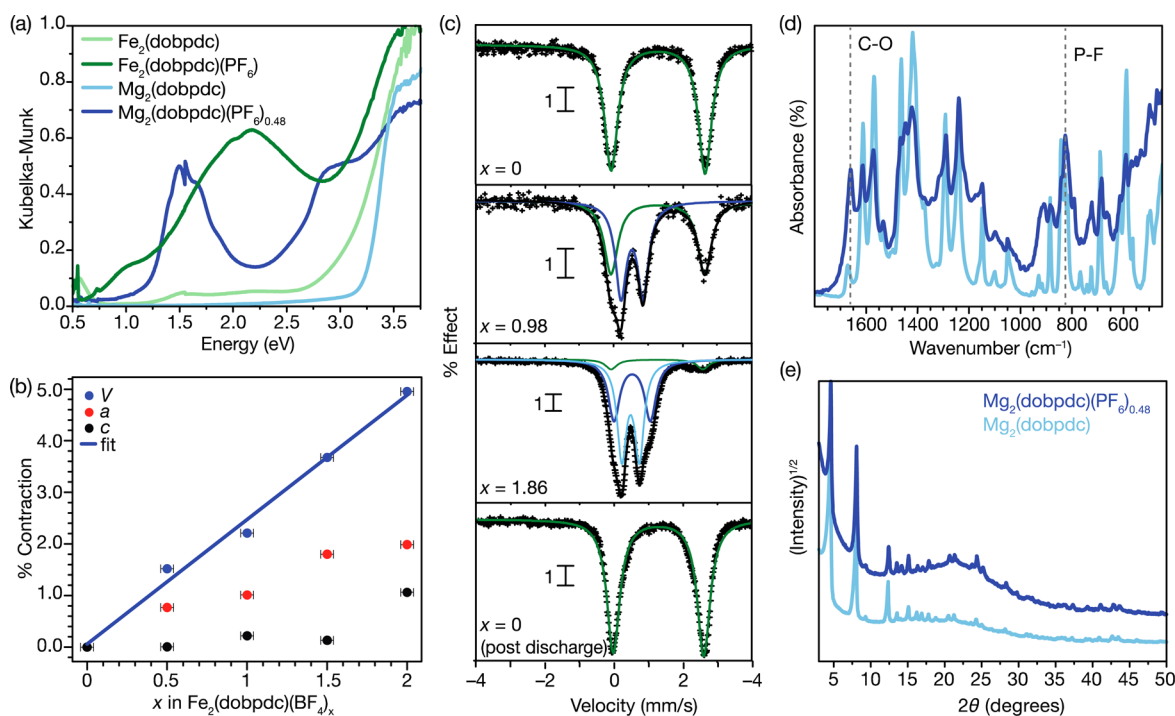
## Supporting Information

Page 13596. It has come to our attention that three Fe-57 Mössbauer spectra in Figure 3 were fitted with the incorrect peak nesting. The spectra shown in Figure 3c for  $\text{Fe}_2(\text{dobpdc})(\text{BF}_4)_x$  ( $x = 0.98$  and  $x = 1.86$ ) have been updated in the corrected version of Figure 3 provided here. Table S9 in the Supporting Information has also been updated with the correct fit parameters.

Page 13597. In the third sentence of the last paragraph of section 2.1, the Mössbauer spectra for  $\text{Fe}_2(\text{dobpdc})(\text{PF}_6)$  discussed were also fitted with the incorrect peak nesting. With the correct fit parameters, this sentence should read as follows: “Upon oxidation to the half-ferric material ( $x = 1$ ) a new doublet

emerges, with  $\delta = 0.535$  mm/s and  $\Delta_E = 0.626$  mm/s, matching those values expected for a high-spin iron(III) center.” Figure S4 and Table S8 in the Supporting Information have also been updated with the corrected fits and fit parameters.

These corrected Mössbauer fit parameters are more consistent with similar high-spin iron(II) and high-spin iron(III) spectra reported in the literature. The newly calculated Fe(II):Fe(III) ratios that result from the corrected fits are statistically indistinguishable from the originally reported values; therefore, these changes do not impact any of the conclusions drawn from the experiment.



**Figure 3.** (a) NIR–vis–UV absorption spectrum for chemically oxidized samples, (b) unit cell parameters determined ex situ powder X-ray diffraction for electrochemically oxidized samples of  $\text{Fe}_2(\text{dobpdc})(\text{BF}_4)_x$  and (c) ex situ  $^{57}\text{Fe}$  Mössbauer spectra for electrochemically oxidized samples of  $\text{Fe}_2(\text{dobpdc})(\text{BF}_4)_x$ , experimental data (+), high-spin iron(II) (green), high-spin iron(III) (blue and light blue), and the fits (black). The values of  $x$  in b and c correspond to  $\text{Fe}_2(\text{dobpdc})(\text{BF}_4)_x$  and were determined electrochemically. Samples were oxidized in three electrode electrochemical cells with lithium counter and reference electrodes and a 0.1 M  $\text{LiBF}_4$  electrolyte in propylene carbonate. (d) Infrared spectra of  $\text{Mg}_2(\text{dobpdc})$  (light blue) and  $\text{Mg}_2(\text{dobpdc})(\text{PF}_6)_{0.48}$  (dark blue) revealed a new C–O stretch ( $1661\text{ cm}^{-1}$ ) and a new P–F stretch ( $823\text{ cm}^{-1}$ ) after oxidation. (e) Powder X-ray diffraction of  $\text{Mg}_2(\text{dobpdc})$  (light blue) and  $\text{Mg}_2(\text{dobpdc})(\text{PF}_6)_{0.48}$  (dark blue) show a 0.9% contraction in unit cell. The very broad feature at  $20^\circ$  originates from the borosilicate glass capillary used to exclude air from the sample.

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## ■ ASSOCIATED CONTENT

### 📄 Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: [10.1021/jacs.5b12875](https://doi.org/10.1021/jacs.5b12875).

Additional details with regard to experimental methods, unit cell refinements, Mössbauer analysis, absorption edge analysis, calculation of ion sizes, iron distances, and discharge curves from the literature (corrected) ([PDF](#))

## ■ ACKNOWLEDGMENTS

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