

Georgia Tech Design in-situ and ex-situ formed coatings to increase the stability of FeF₃ Na-ion cathodes

Zifei Sun, Peilin Lu, Wenbin Fu, Baichuan Wang, Alexandre Magasinski, Yawei Zhang and Prof. Gleb Yushin*

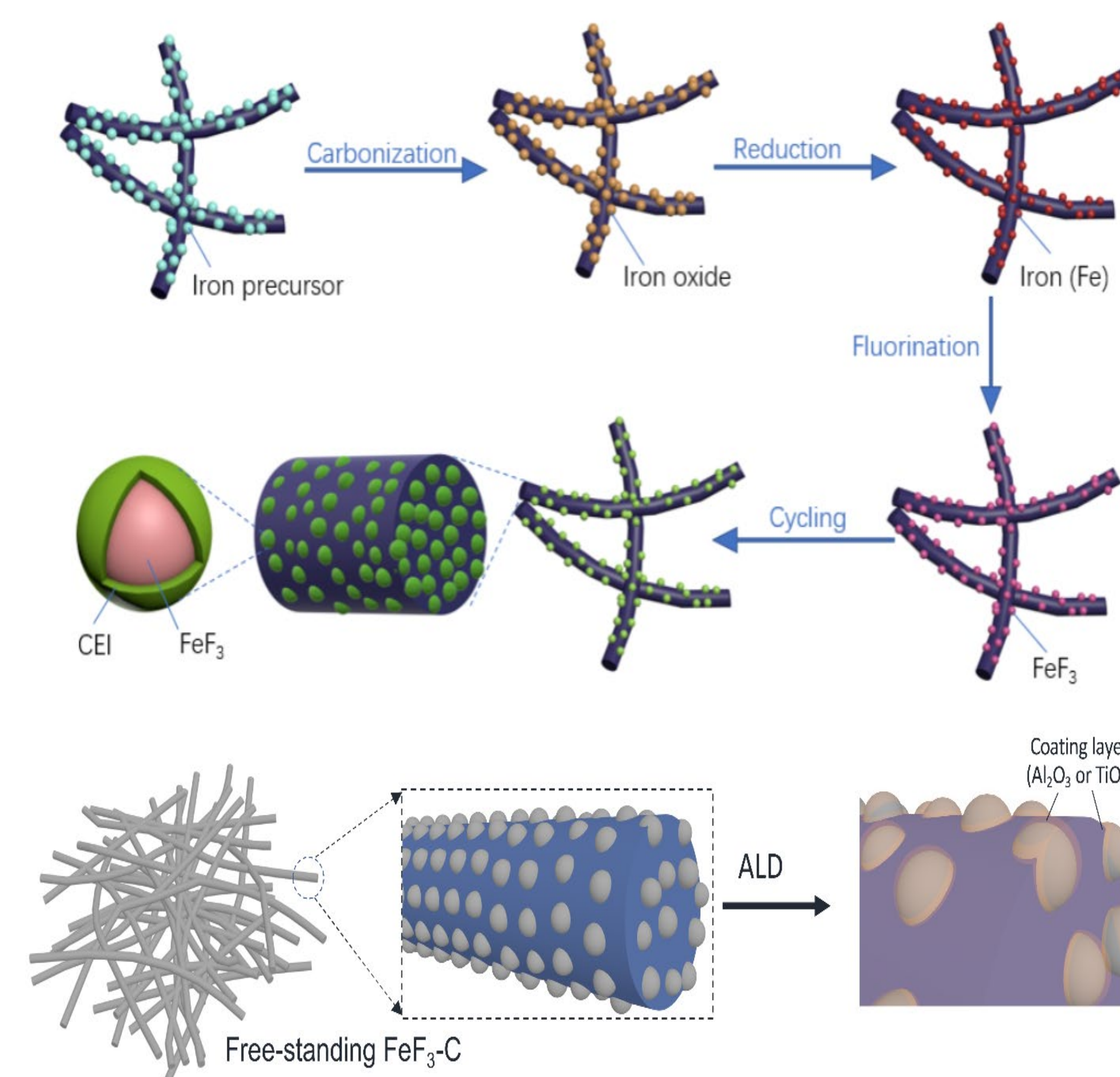
Georgia Institute of Technology | Department of Chemistry and Biochemistry, Department of Materials Science and Engineering | 771 Ferst Drive NW Atlanta, GA 30332 USA
yushin@gatech.edu; www.nano-tech.gatech.edu

MOTIVATION

- Sodium-ion batteries(NIBs) as a potential alternative to lithium-ion batteries have attracted great attention due to their low cost and high abundance.
- Iron trifluoride (FeF₃) has been explored enthusiastically due to its low cost, great abundance and high theoretical capacity (712mAh/g).
- However, FeF₃ tends to dissolve during charging and discharging. Further input needs to improve the stability of FeF₃-based cathode materials.
- Herein, we designed in-situ formed protective layers by electrode and electrolyte interaction and ex-situ formed protective layers by atomic layer deposition (ALD) technique.

ELECTRODE FABRICATION

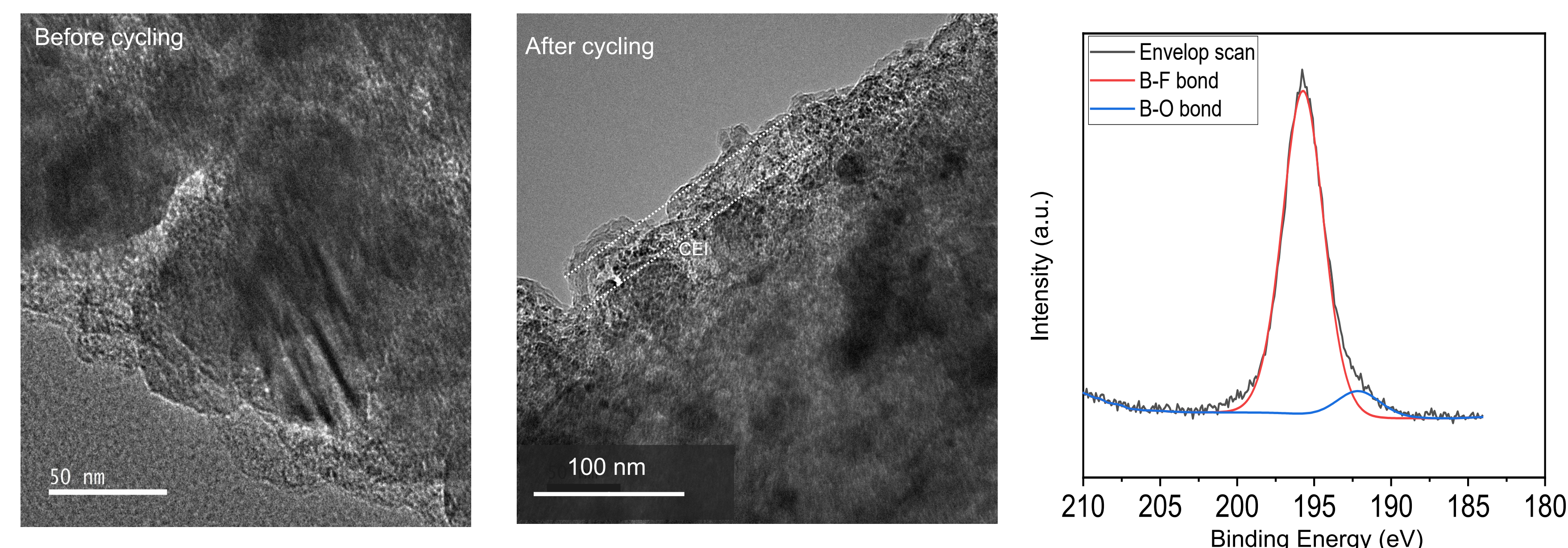
- Electrospinning is used to synthesize FeF₃-Carbon nanofibers (CNFs).



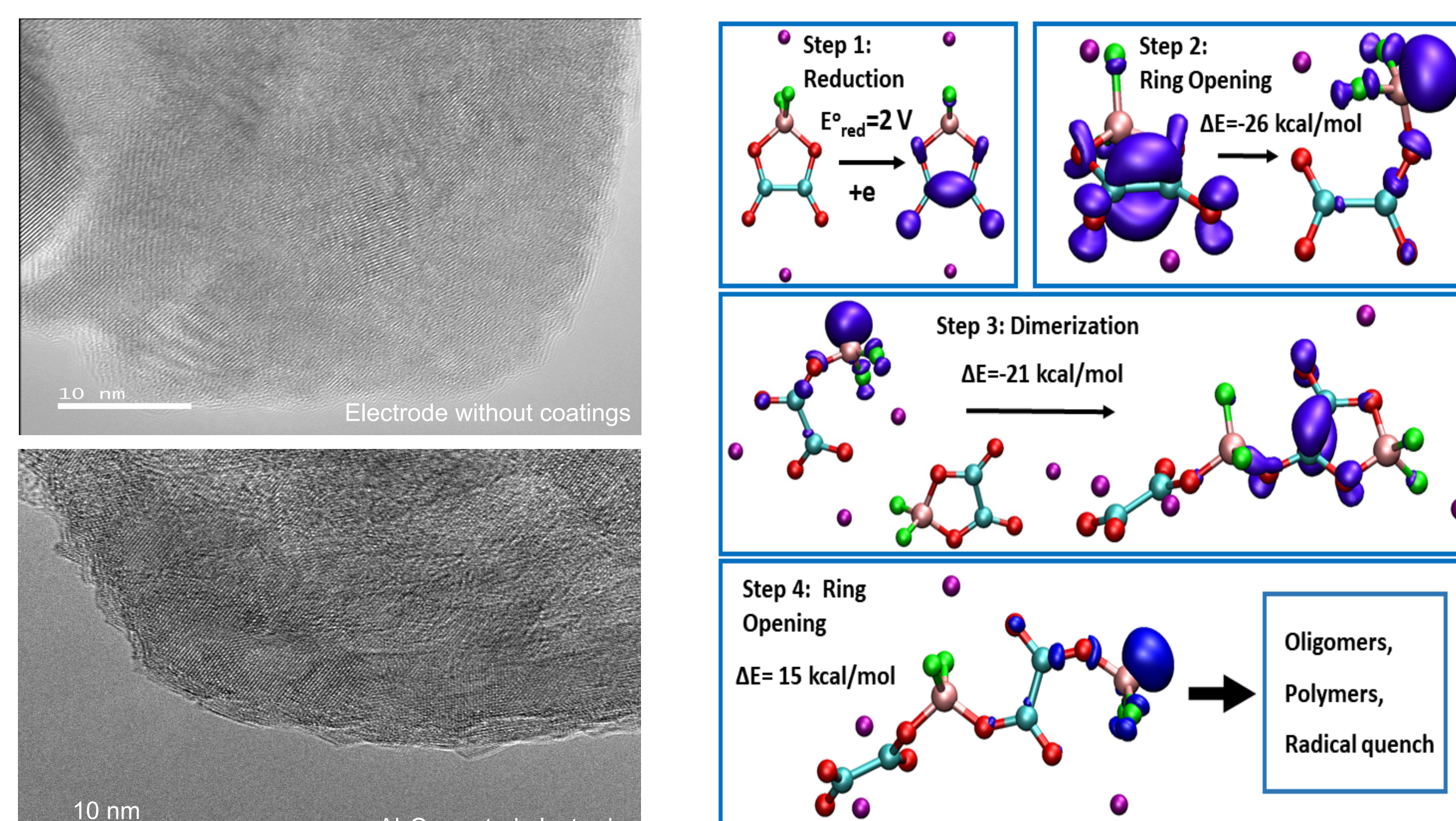
- This approach increases the electrical conductivity and ionic conductivity.
- Conformal alumina (Al₂O₃) ALD coatings are deposited at the surface of cathodes.

CHARACTERIZATION OF DESIGNED COATINGS

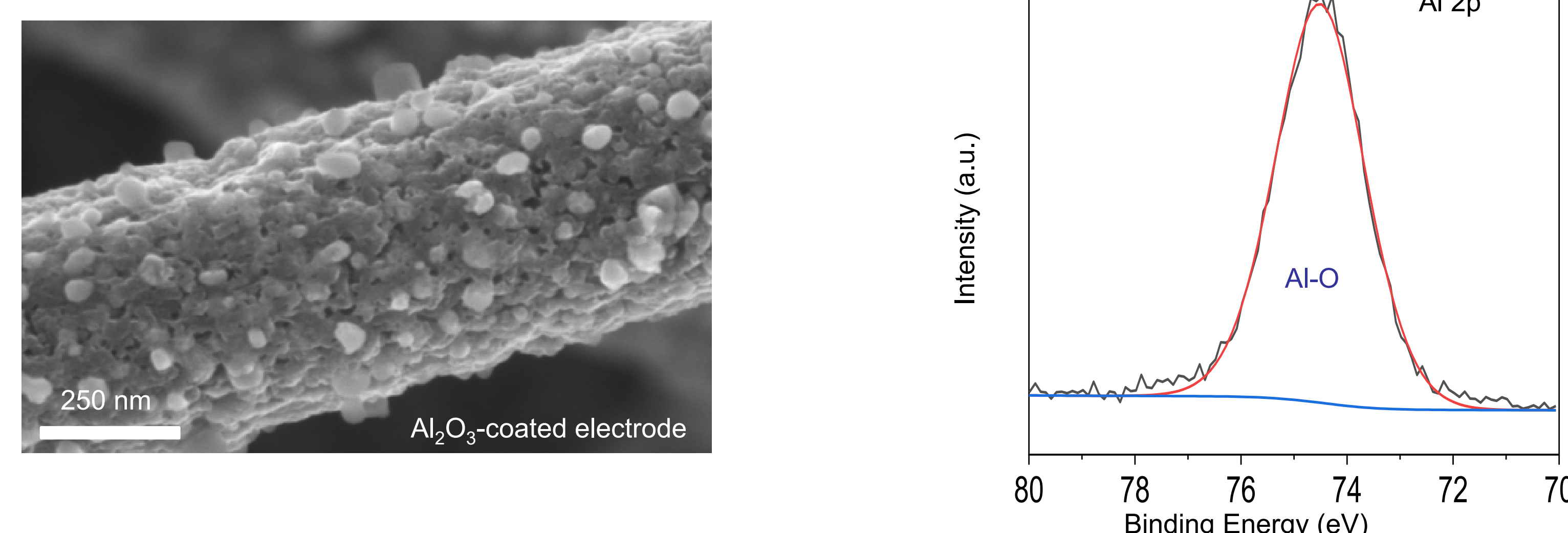
- A in-situ formed protective coating called cathode electrolyte interphase (CEI) was successfully fabricated by the electrochemical reaction.
- XPS of B_{1s} spectra shows the existence of B-F and B-O bonds inside of CEI.



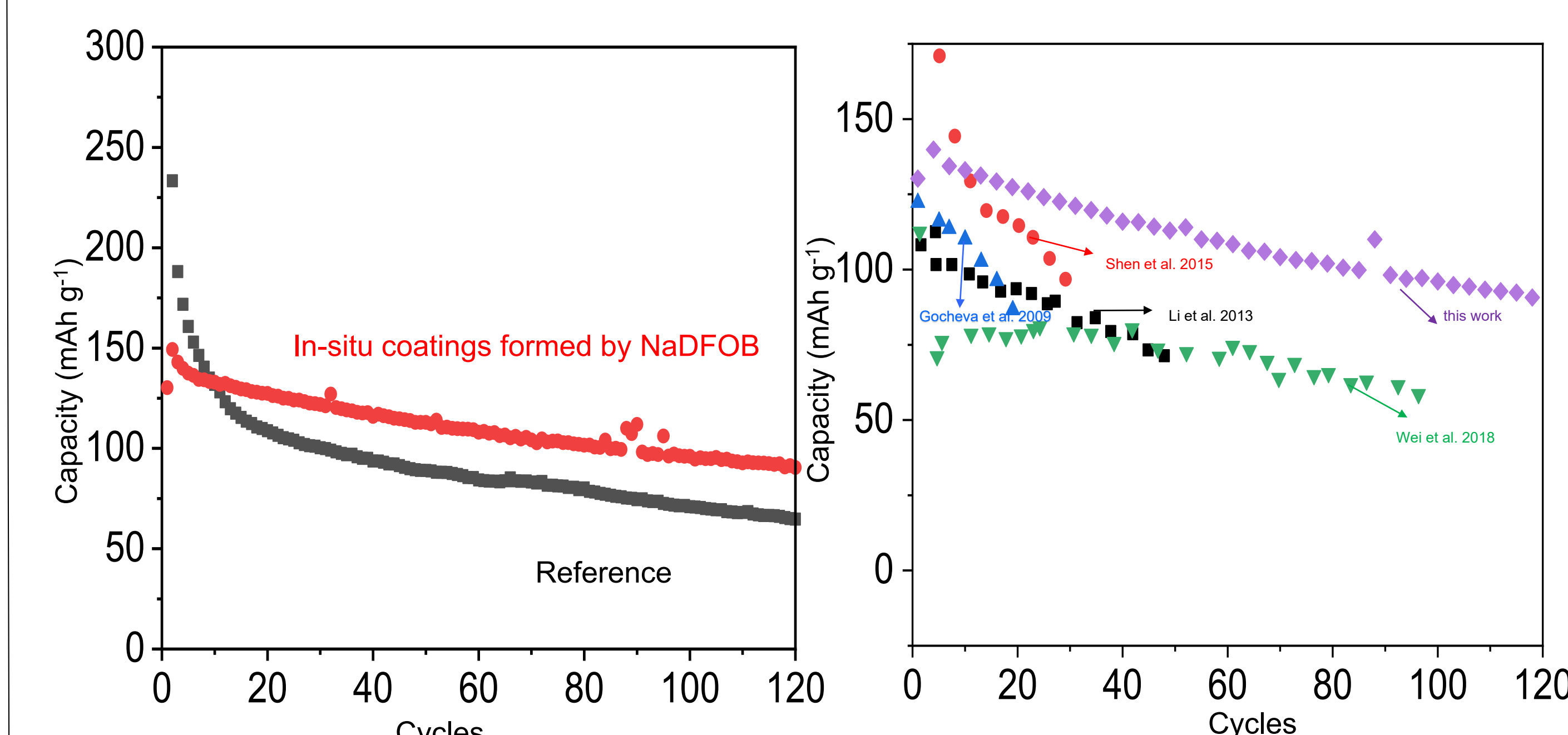
- Quantum mechanics reveal the CEI was initiated by the Na⁺-mediated dimerization of electrolyte salt (NaDFOB). Further oligomerization would proceed through analogous steps.



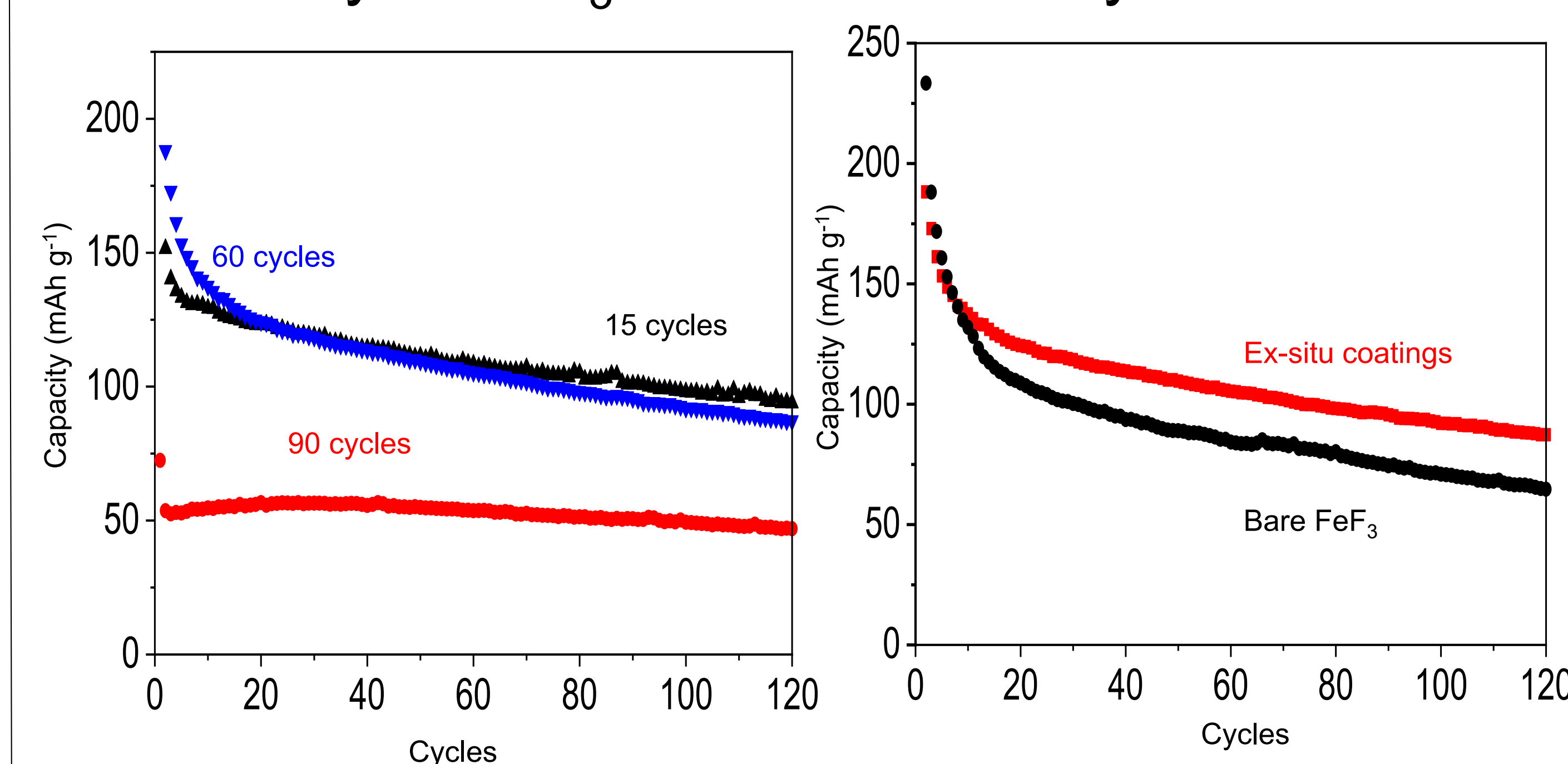
- Al₂O₃ was selected as the ALD coating layers and deposited on the cathode surface for ex-situ formed protective layers.



ELECTROCHEMICAL PERFORMANCE



- In-situ formed coatings improved the cycling stability of FeF₃ in the first 120 cycles.



- Ex-situ formed coatings improved the cycling stability of FeF₃ in the first 120 cycles and 15 ALD Al₂O₃ coatings performed the best when comparing coatings with other ALD cycles.

CONCLUSION

- In-situ formed protective coatings were successfully designed and showed good performance to improve the cycling performance.
- In-situ coatings were formed by polymerization of DFOB anion during cycling.
- Ex-situ coatings were successfully fabricated by ALD technique.
- 15 ALD cycles for Al₂O₃ coatings exhibited the best cycling performance among coatings with other ALD cycles.

ACKNOWLEDGEMENTS

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Disclosure: A nanowire patent has been licensed to Sila Nanotechnologies, Inc.; G. Yushin is a co-founder, BOD member and stock holder of Sila.



REFERENCE

- [1] Z. Sun, W. Fu, M. Liu, P. Lu, E. Zhao, A. Magasinski, M. Liu, S. Luo, J. McDaniel, G. Yushin, *Journal of Materials Chemistry*, **2020**, 8, 4091.
- [2] W. Fu, E. Zhao, Z. Sun, X. Ren, A. Magasinski, G. Yushin, *Advanced Functional Materials* **2018**, 28, 1801711.
- [3] E. Zhao, O. Borodin, X. Gao, D. Lei, Y. Xiao, X. Ren, W. Fu, A. Magasinski, K. Turcheniuk, G. Yushin, *Advanced Energy Materials* **2018**, 8, 1800721.