Supporting Information

Synergistic effect on electrochemical performance of LiFePO₄ Cathodes *via* carbon coating and Ni²⁺ Doping: A Combined Experimental and Theoretical Approach

Shreyas J. Kashyap^{a, b}, Ch. Gowthami^a, Sougat Purohit^c, Gopalakrishnan Sai Gautam^c Vadali V S S Srikanth^b, R. Vijay^a, Tata N. Rao^d, S. Anandan^{a, *}

^aCentre for Nanomaterials, International Advanced Centre for Powder Metallurgy and New Materials (ARCI), Balapur, Hyderabad 500005, Telangana, India

^bSchool of Engineering Sciences and Technology, University of Hyderabad, Hyderabad 500046, Telangana, India

^cDepartment of Materials Engineering, Indian Institute of Science, Bengaluru, Karnataka 560012, India

^dDepartment of Materials Science & Metallurgical Engineering, Indian Institute of Technology, Hyderabad 502285, India

*Corresponding author e-mail: <u>anandan@arci.res.in</u>

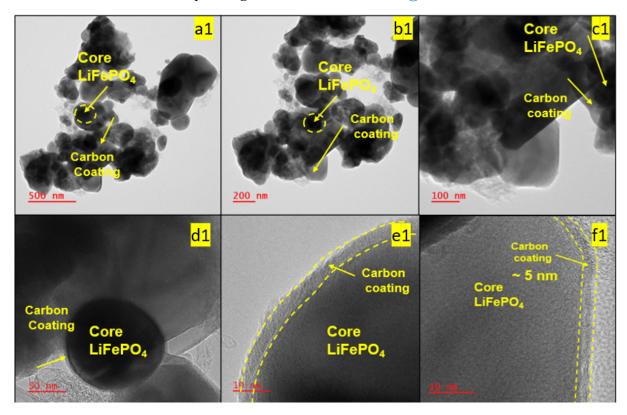


Fig.S1: HR-TEM images of Ni-LFP/C with optimum carbon content.

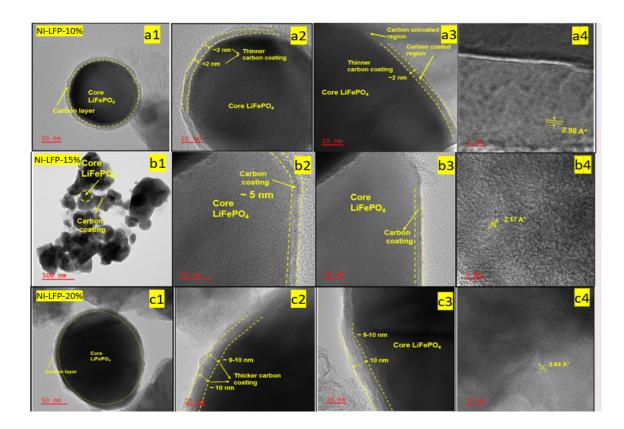


Fig.S2: HR-TEM images of Ni-LFP/C with different concentration of carbon precursor (a1-a4) Ni-LFP with 10 wt% carbon precursor, (b1-b4) Ni-LFP with 15wt% carbon precursor, (c1-c4) Ni-LFP with 20 wt% carbon precursor

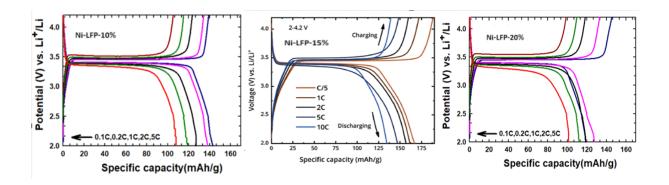


Fig S3. Charge-discharge profiles of Ni-LFP/C with different concentration of carbon precursor measured at different C-rate.

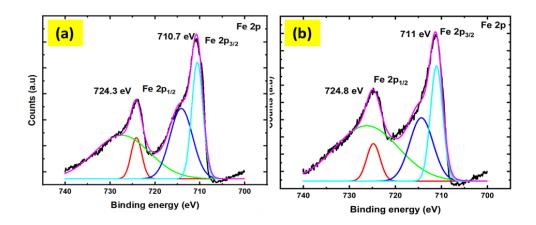


Fig S4. Deconvoluted XPS core-level Fe 2p spectra of LiFePO₄/C, (a) and Ni-doped LiFePO₄/C (b)

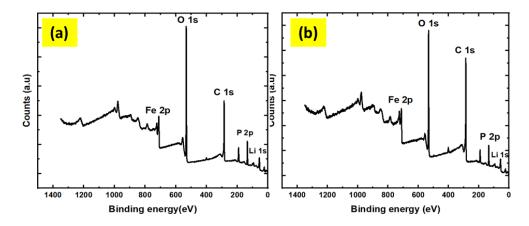


Fig S5. XPS Survey spectrum of LiFePO₄/C (a) and Ni-doped LiFePO₄/C (b)

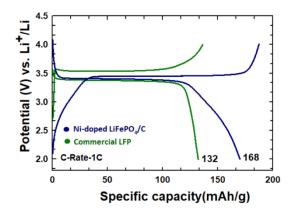


Fig S6: Benchmarking studies of Ni²⁺ doped LFP/C (Charge-Discharge) measured at 1C

Dopant	Capacity @ C-rate	Reference
Ti ⁴⁺	156 mAh/g @ 1C	[1]
Na ⁺	140 mAh/g @1C	[2]
F-	159.3 mAh/g @ 1C	[3]
Mg^{2+}	142 mAh/g @ 1C	[4]
Ni ²⁺	141 mAh/g @ 1C	[5]
Ni ²⁺	166 mAh/g @ 1C	This work

Table S1: Comparison of electrochemical performance of doped LiFePO₄ cathode material with state of art literature

References

- [1] L. Yang, Y. Tian, J. Chen, J. Gao, Z. Long, W. Deng, G. Zou, H. Hou, X. Ji, A high-rate capability LiFePO 4 /C cathode achieved by the modulation of the band structures, J Mater Chem A Mater 9 (2021) 24686–24694. https://doi.org/10.1039/D1TA07757K.
- [2] Y. Liu, W. Qin, D. Zhang, L. Feng, L. Wu, Effect of Na+ in situ doping on LiFePO4/C cathode material for lithium-ion batteries, Progress in Natural Science: Materials International 31 (2021) 14–18. https://doi.org/10.1016/j.pnsc.2020.10.006.
- [3] X. Wang, Z. Feng, X. Hou, L. Liu, M. He, X. He, J. Huang, Z. Wen, Fluorine doped carbon coating of LiFePO4 as a cathode material for lithium-ion batteries, Chemical Engineering Journal 379 (2020) 122371. https://doi.org/10.1016/j.cej.2019.122371.
- [4] X. Liu, Y. Zhang, Y. Meng, T. Kang, H. Gao, L. Huang, F. Zhu, Influence Mechanism of Mg ²⁺ Doping on Electrochemical Properties of LiFePO ₄ Cathode Materials, ACS Appl Energy Mater 5 (2022) 8452–8459. https://doi.org/10.1021/acsaem.2c00986.
- [5] A. Örnek, E. Bulut, M. Can, M. Özacar, Characteristics of nanosized LiNi x Fe1–x PO4/C (x = 0.00–0.20) composite material prepared via sol–gel-assisted carbothermal reduction method, Journal of Solid State Electrochemistry 17 (2013) 3101–3107. https://doi.org/10.1007/s10008-013-2201-5.