

Supporting Information for Publication

**LiMn<sub>2</sub>O<sub>4</sub> Cathode with F Anions Doping for Superior Performance of Lithium-ion  
Batteries**

Zijing Wan, Xiaoxue Jiang, Dongwei Xu,<sup>\*</sup> and Xiaobing Luo

*State Key Laboratory of Coal Combustion, School of Energy and Power Engineering,  
Huazhong University of Science and Technology, Wuhan, Hubei 430074, China.*

(Dated: August 22, 2022)

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\* correspondence to: [dwxu@hust.edu.cn](mailto:dwxu@hust.edu.cn)

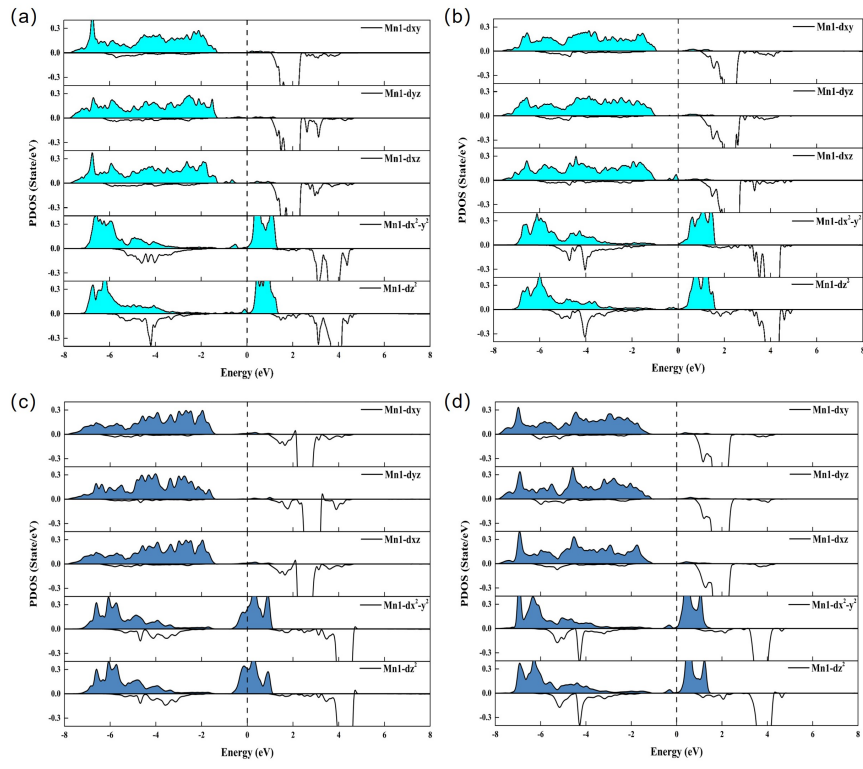


FIG. S1. PDOS of five Mn1-3d orbitals of (a-b)  $\text{Li}_x\text{Mn}_2\text{O}_{3.875}\text{F}_{0.125}$  and (c-d)  $\text{Li}_x\text{Mn}_2\text{O}_4$  in the delithiation process ( $x=0.25, 0.75$ ).

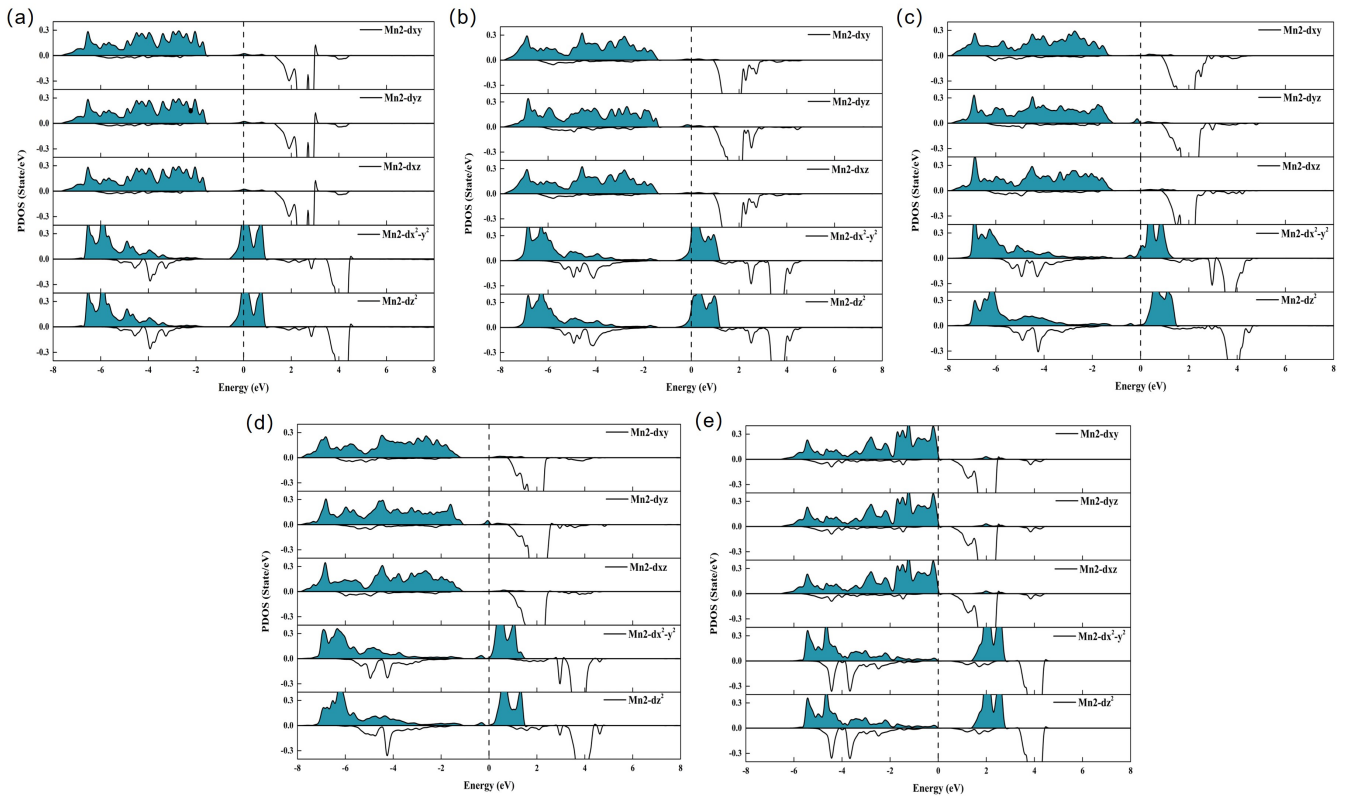


FIG. S2. (a-e) PDOS of five Mn2-3d orbitals of Li<sub>x</sub>Mn<sub>2</sub>O<sub>4</sub> in the delithiation process ( $x=0, 0.25, 0.5, 0.75, 1$ ).

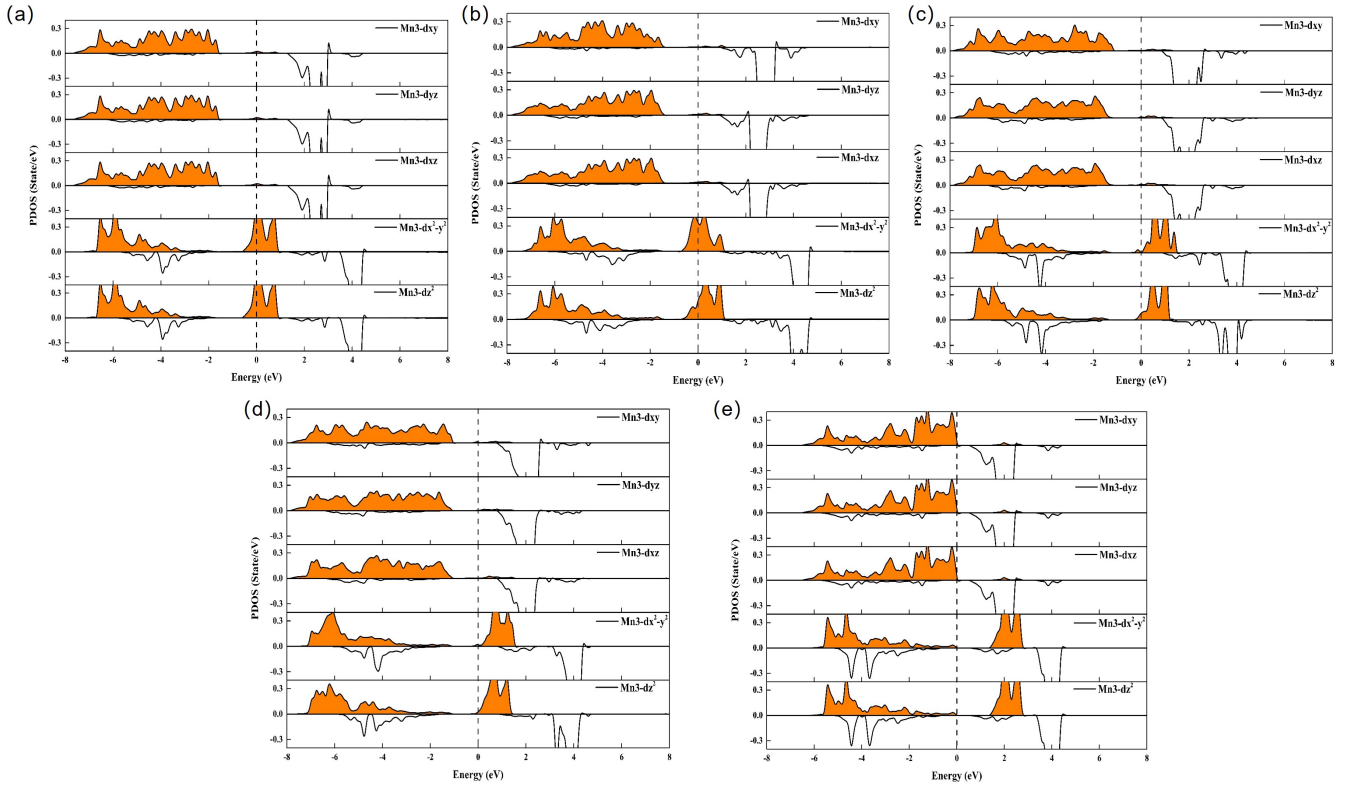


FIG. S3. (a-e) PDOS of five Mn3-3d orbitals in Li<sub>x</sub>Mn<sub>2</sub>O<sub>4</sub> in the delithiation process ( $x=0, 0.25, 0.5, 0.75, 1$ ).

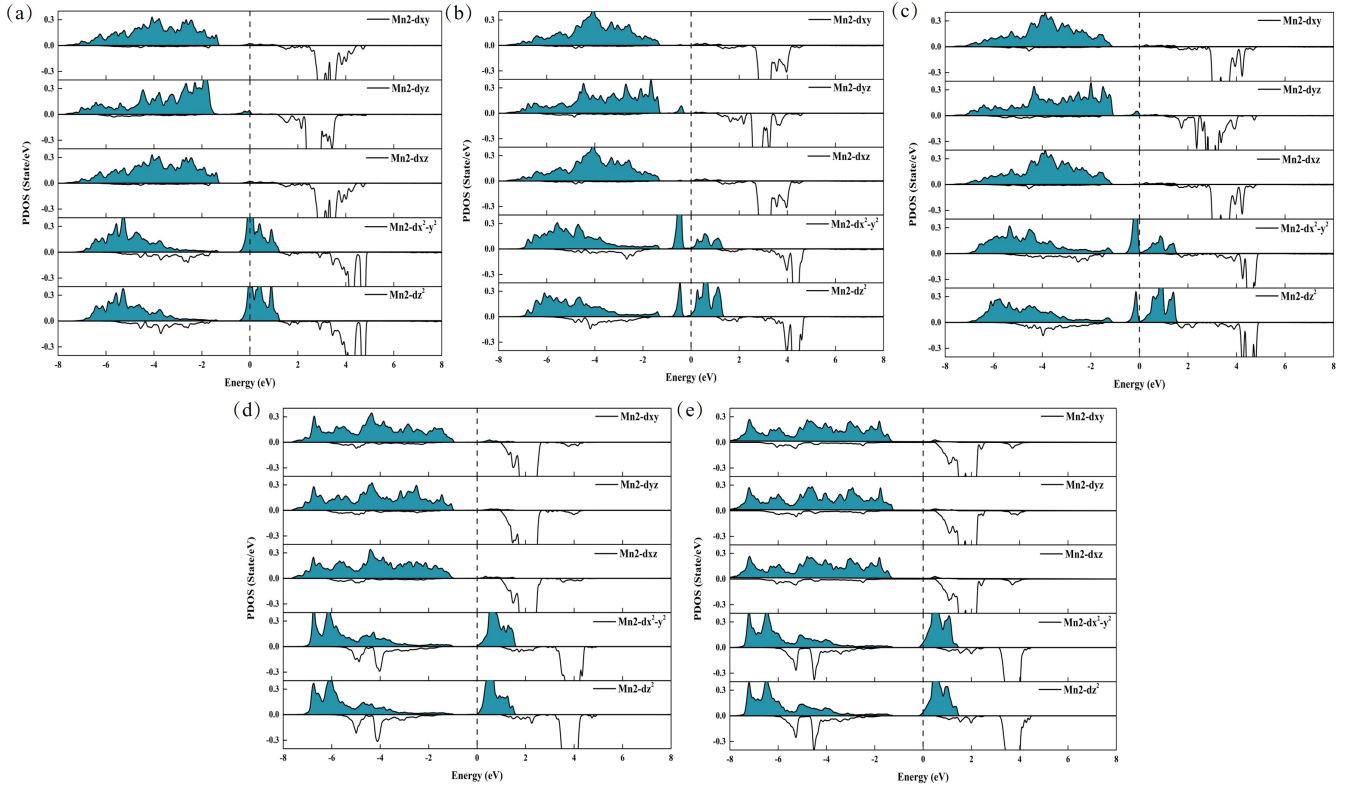


FIG. S4. (a-e) PDOS of five Mn2-3d orbitals of  $\text{Li}_x\text{Mn}_2\text{O}_{3.875}\text{F}_{0.125}$  in the delithiation process ( $x=0, 0.25, 0.5, 0.75, 1$ ).

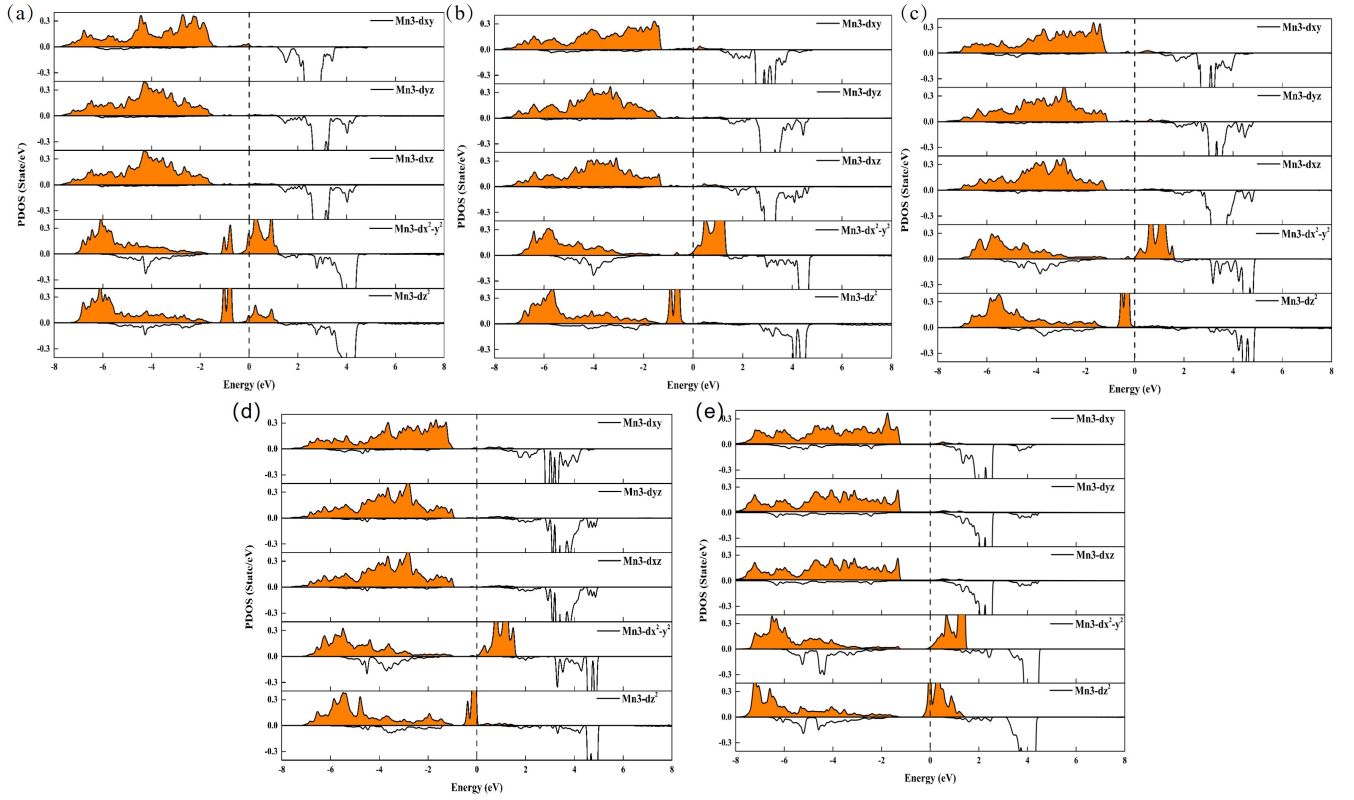


FIG. S5. (a-e) PDOS of five Mn3-3d orbitals of  $\text{Li}_x\text{Mn}_2\text{O}_{3.875}\text{F}_{0.125}$  in the delithiation process ( $x=0, 0.25, 0.5, 0.75, 1$ ).

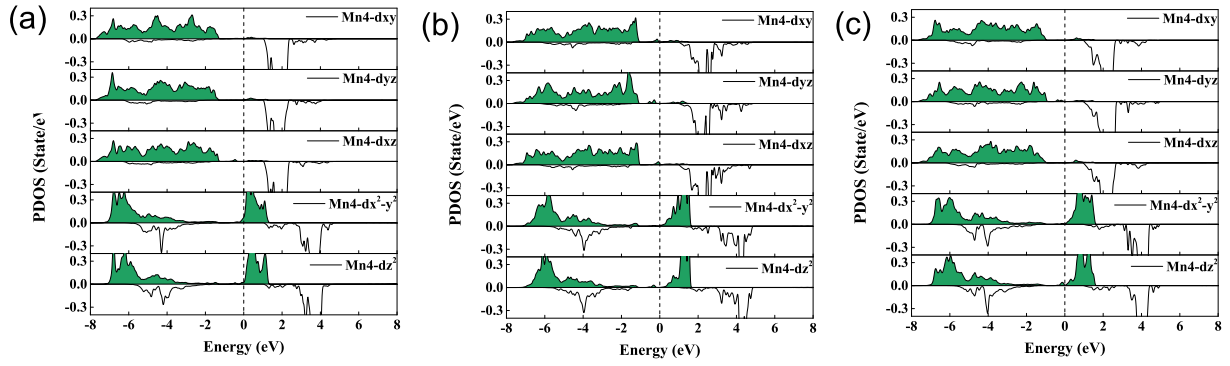


FIG. S6. (a-c)PDOS of five Mn4-3d orbitals in  $\text{Li}_x\text{Mn}_2\text{O}_{3.875}\text{F}_{0.125}$  in the delithiation process at  $x=0.75, 0.5,$  and  $0.25$ .

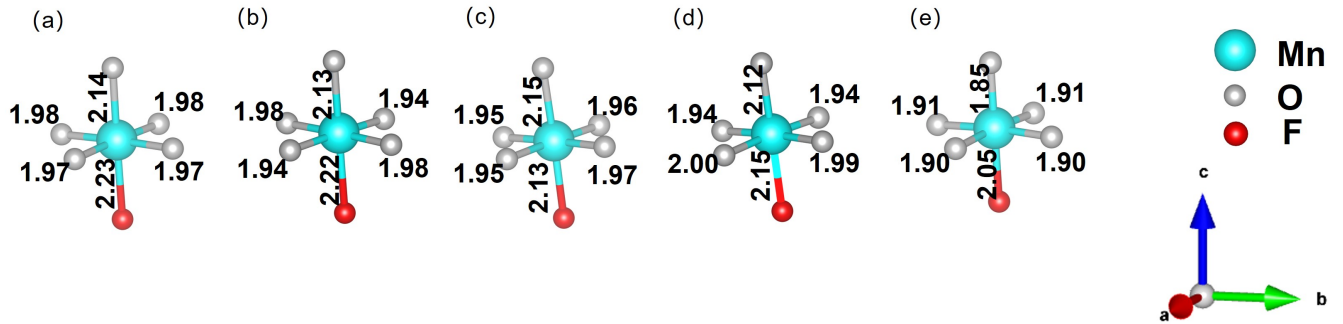


FIG. S7. (a-e) The ball and stick model of Mn3-O octahedron of  $\text{Li}_x\text{Mn}_2\text{O}_{3.875}\text{F}_{0.125}$  in the delithiation process ( $x=0, 0.25, 0.5, 0.75, 1$ ). The cyan, grey, red spheres represent Mn, O and F atoms respectively.