Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.


# High rates $Na_{0.7}Li_{2.3}V_2(PO_4)_2F_3$ hollow sphere cathode for lithium ion battery, prepared via solvothermal and electrochemical ion exchange

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**$N_{0.7}$VPF**

a=8.8521 Å, b=8.8631 Å, c=10.9985 Å

α=β=γ=90°

Volume of unit cell: 862.9098 $Å^3$

| Atom | x | y | z | Occupancy |
|---|---|---|---|---|
| **Na1** | 0.009 (2) | 0.195 (4) | 0.500000 | 1 |
| **V1** | 0.359 | 0.258 (2) | 0.189 (5) | 1 |
| **V2** | 0 | 0.249 (3) | 0.183 (6) | 1 |
| **P** | 0.25 | 0.501 (7) | 0.343 (9) | 1 |
| **O1** | 0.309 (9) | 0.099 (7) | 0.280 (3) | 1 |
| **O2** | 0.305 (5) | 0.515 (3) | 0.356 (9) | 1 |
| **O3** | 0.144 (8) | 0.104 (8) | 0.145 (2) | 1 |
| **O4** | 0.159 (7) | 0.425 (4) | 0.203 (5) | 1 |
| **F1** | 0.5 | 0.291 (2) | 0.835 (6) | 1 |
| **F2** | 0.5 | 0.0420 (8) | 0.010 (3) | 1 |
| **F3** | 0.5 | 0.275 (6) | 0.251 (7) | 1 |

**$N_{0.7}Li_{2.3}VPF$**

a=9.1899Å, b=9.2158Å, c=10.9746Å

α=β=γ=90°

Volume of unit cell: 929.4639 $Å^3$

| Atom | x | y | z | Occupancy |
|---|---|---|---|---|
| **Li0** | 0.039 (2) | 0.276 (2) | 0.500 | 1 |
| **Li1** | 0.264 (5) | 0.485 (1) | 0.500 | 1 |
| **Li2** | 0.235 (3) | 0.583 (5) | 0.500 | 1 |
| **V12** | 0.241 (7) | 0.237 (6) | 0.192 (5) | 1 |
| **P20** | 0.000 | 0.000 | 0.231 (6) | 1 |
| **P21** | 0.000 | 0.500 | 0.149 (5) | 1 |
| **O30** | 0.015 (2) | 0.065 (5) | 0.748 (9) | 1 |
| **O32** | 0.153 (7) | 0.965 (9) | 0.610 (5) | 1 |
| **O34** | 0.085 (8) | 0.463 (6) | 0.831 (7) | 1 |
| **F60** | 0.349 (3) | 0.176 (8) | 0.375 | 1 |
| **F62** | 0.196 (7) | 0.479 (9) | 0.000 | 1 |

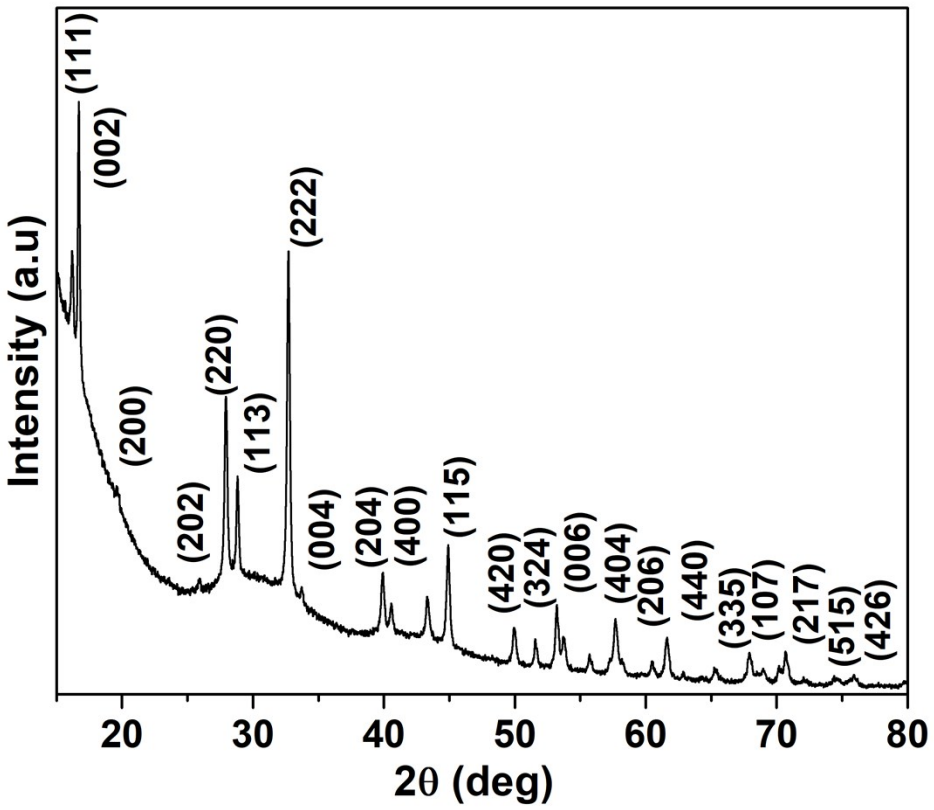


***Figure S1 XRD pattern of NVPF***

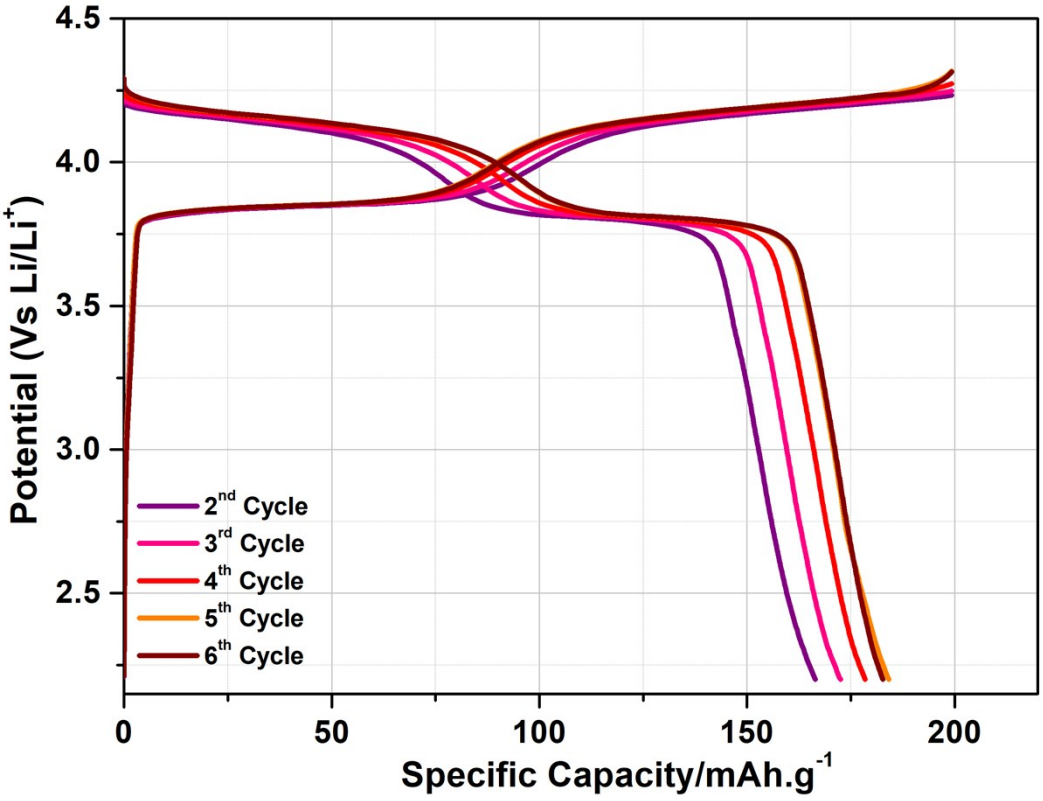


*Figure S2 First 5 stabilization cycles*

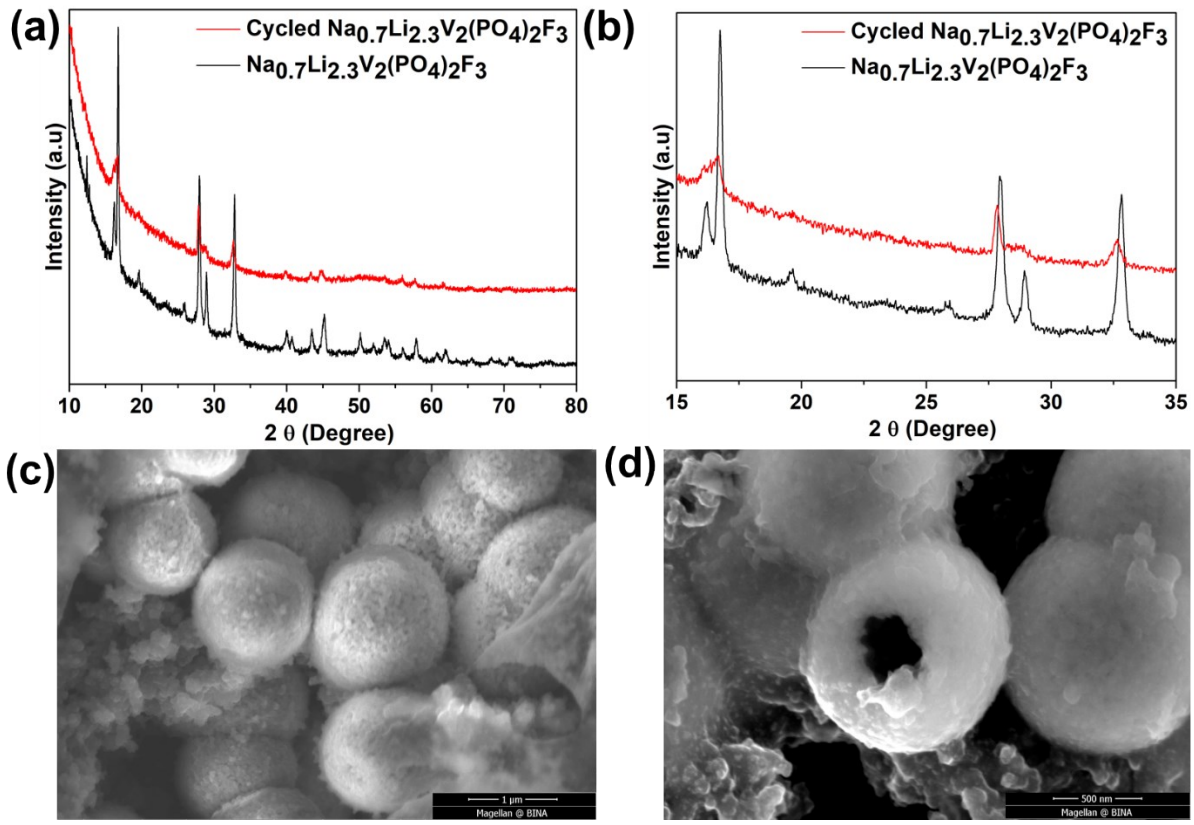


***Figure S3 XRD pattern of $N_{0.7}$ $L_{2.3}V_2PF$ electrode before and after electrochemical cycling in (a) 2Θ = 10°-80°, (b) 2Θ = 15°-35°, (c)Low magnification and (d) high magnification HRSEM images of $N_{0.7}$ $L_{2.3}V_2PF$ electrode after electrochemical cycling***