

Sodium-Ion Battery Cathodes $\text{Na}_2\text{FeP}_2\text{O}_7$ and $\text{Na}_2\text{MnP}_2\text{O}_7$: Diffusion Behaviour for High Rate Performance

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Supplementary Information

Table S1. Interatomic potentials and shell model parameters for $\text{Li}_2\text{FeP}_2\text{O}_7$ and $\text{Na}_2\text{MP}_2\text{O}_7$ ($M = \text{Fe}, \text{Mn}$).

Buckingham			
Interaction	A (eV)	ρ (Å)	C (eV·Å ⁶)
Li ⁺ - O ²⁻	632.1018	0.2906	0.0
Na ⁺ - O ²⁻	1497.830598	0.28743	0.0
Fe ²⁺ - O ²⁻	1105.2409	0.3106	0.0
Mn ²⁺ - O ²⁻	3248.3500	0.2690	0.0
P ⁵⁺ - O ²⁻	1029.0500	0.3470	0.0
O ²⁻ - O ²⁻	22764.3	0.1490	44.53
Shell model			
Species	Y (e)	k (eV·Å ⁻²)	
Fe ²⁺	2.997	19.26	
Mn ²⁺	3.42	95.00	
O ²⁻	-2.96	65.0	