

NFMO Na-ion Battery Cathodes: From Structural ‘Anatomy’ to Redox Mechanism

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The Ca-doped and undoped $\text{Na}_x[\text{Fe}_{1/2}\text{Mn}_{1/2}]\text{O}_2$ (NFMO) Na-ion battery cathode material is currently under investigation within the international project GENSIB (*Genetic Approach to Sodium-Ion Batteries*) at the Department of Low Temperature Physics and at the institutions of the other project partners. Recent progress in understanding the ‘anatomy’ of NFMO—its atomic, electronic, and magnetic structure—is reviewed. This framework guides our tentative explanation of the redox orbitals likely active in Na-ion NFMO batteries, recognizing that their precise identification remains under debate. The project combines multiple theoretical/numerical and experimental methods—including redox orbital analysis—warranting study complementarity.