

Coordination compounds in lithium storage and lithium-ion transport

Jingwei Liu, Daixi Xie, Wei Shi* and Peng Cheng*

Key Laboratory of Advanced Energy Materials Chemistry (MOE), College of Chemistry, Nankai

University, Tianjin 300071, China

Email: shiwei@nankai.edu.cn; pcheng@nankai.edu.cn

Table S1 Electrochemical reaction mechanisms, potentials, and theoretical capacities of representative electrode materials for LIBs

Electrodes	Materials	Reaction mechanism	Voltage ^a (V)	Capacity ^b (mA h g ⁻¹)	Advantages	Disadvantages	Ref.
Cathode	Organic materials (1,4-benzoquinone)	$C_6H_4O_2 + 2Li^+ + 2e^- \leftrightarrow Li_2C_6H_4O_2$	2.7	495	High capacity and low cost	High solubility and low conductivity	13
	Lithium-rich layered oxides (Li _{1+x} M _{1-x} O ₂ , M = Mn, Ni, Co)	$LiCoO_2 \leftrightarrow CoO_2 + Li^+ + e^-$	3.7	274	High volumetric energy density	High cost, poor cycling stability	15
	Polyanionic compounds (LiFePO ₄)	$LiFePO_4 \leftrightarrow FePO_4 + Li^+ + e^-$	3.45	170	High stability and cyclability	Low conductivity	16
	Spinel oxides (LiMn ₂ O ₄)	$LiMn_2O_4 \leftrightarrow 2MnO_2 + Li^+ + e^-$	4.0	150	Fast kinetics	High solubility in the electrolyte	15
	Nickel-rich layered oxides (LiNi _{1-x} M _x O ₂ , M = Co, Mn and Al)	$LiNi_{0.5}Mn_{1.5}O_2 \leftrightarrow Ni_{0.5}Mn_{1.5}O_2 + Li^+ + e^-$	4.7	146	High operating voltage	Poor cycling and thermal stability	16
Anode	Conversion-type (Transition metal oxides)	$Fe_2O_3 + 6Li^+ + 6e^- \leftrightarrow 2Fe + 3Li_2O$	0.9	1005	High capacity	Large structural change and low conductivity	15
	Alloying-type (Si, Sn, P)	$Sn + 4.4Li^+ + 4.4e^- \leftrightarrow Li_{4.4}Sn$	0.5	990	High capacity and low potential	Massive volume variation	17
	Insertion-type (Graphite, Li ₄ Ti ₅ O ₁₂)	$6C + Li^+ + e^- \leftrightarrow LiC_6$	0.1	370	Fast kinetics and high abundance	Low capacity	3
	Organic materials (Conjugated carboxylates)	$Li_2C_8H_4O_4 + 2Li^+ + 2e^- \leftrightarrow Li_4C_8H_4O_2$ (insertion reaction)	0.85	301	Fast kinetics	High solubility and low conductivity	13

^a Average discharge voltage (vs. Li⁺/Li); ^b theoretical capacity.