

Supporting information

Electrochemical reactions in fluoride-ion batteries: mechanistic insights from Pair Distribution Function analysis

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Phase name	Crystal system	Space group	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	Ref./ICSD Coll. Code
La _{0.95} Ba _{0.05} F _{2.95}	Trigonal	<i>P</i> -3 <i>c</i> 1	7.20	7.20	7.37	90	90	120	Rongeat <i>et al.</i> ¹
La _{0.95} Ba _{0.05} F _{2.95}	Trigonal	<i>P</i> -3 <i>c</i> 1	7.207	7.207	7.373	90	90	120	Chable <i>et al.</i> ²
LaF ₃	Trigonal	<i>P</i> -3 <i>c</i> 1	7.185	7.185	7.351	90	90	120	23972
Bi	Trigonal	<i>R</i> -3 <i>m</i>	4.546	4.546	11.862	90	90	120	64703
α-Bi ₂ O ₃	Monoclinic	<i>P</i> 21/ <i>c</i>	5.844	8.157	7.503	90	113	90	94229
β-BiF ₃	Orthorhombic	<i>Pnma</i>	6.561	7.015	4.841	90	90	120	1269
α-BiF ₃	Cubic	<i>Fm</i> -3 <i>m</i>	5.861	5.861	5.861	90	90	90	Hund and Frick ³ /24522
β-BiO _x F _{3-2x}	Cubic	<i>Fm</i> -3 <i>m</i>	5.848	5.848	5.848	90	90	90	Morell <i>et al.</i> ⁴
BiO _{0.1} F _{2.8}	Hexagonal	<i>P</i> 63/ <i>mmc</i>	4.083	4.083	7.323	90	90	120	24056
BiO _{0.55} F _{1.9} c-BiO _x F _{3-2x}	Trigonal	<i>R</i> -3 <i>m</i>	4.138	4.138	20.321	90	90	120	Laval <i>et al.</i> ⁵ /50823
Bi ₇ F ₁₁ O ₅	Monoclinic	<i>C</i> 121	13.524	5.529	9.189	90	96	90	167074
BiOF	Tetragonal	<i>P</i> 4/ <i>nmm</i>	3.747	3.747	6.226	90	90	90	24096

Table S1. Crystallographic data relevant to the study of the Bi-BiF₃ composite electrodes. Please refer to the corresponding reference or ICSD collection code for more details. a, b and c represent the lattice parameters and α, β and γ the lattice angles.

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