Ionic transport and luminescence properties in sodium- and fluorine-co-doped rare-earth molybdates $NaLn_4Mo_3O_{15}F$ (*Ln* = Sm–Tb)

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Supplementary materials

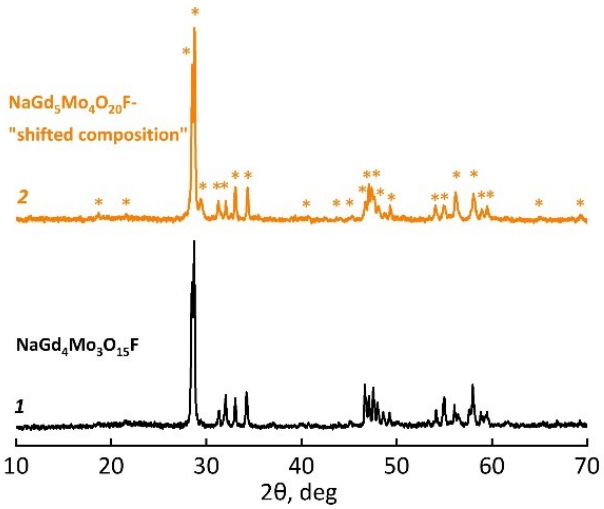

Figure S1. XRD patterns of polycrystalline samples: (1) $NaGd_4Mo_3O_{15}F$ sample, synthesized at 700 °C in vacuum; (2) reduced $NaGd_5Mo_4O_{20}F$ sample, synthesized at 700 °C in vacuum. The asterisk symbol marks the reflections of the Gd_2MoO_6 phase.

Table S1. Refined atomic positions in the $NaSm_4Mo_3O_{15}F$ structure.

Atom	x	y	z	Occupancy
Sm1	0.0000	0.0000	0.0000	1.0
Sm2	0.9978	0.2500	0.2500	0.6667
Na1	0.9978	0.2500	0.2500	0.3333
Mo1	0.0000	0.7500	0.2500	1.0
O1	0.3349	0.1151	0.9143	0.9166
O2	0.1714	0.1714	0.1714	1.0
F1	0.3349	0.1151	0.9143	0.0834

Table S2. Refined atomic positions in the $NaEu_4Mo_3O_{15}F$ structure.

Atom	x	y	z	Occupancy
Eu1	0.0000	0.0000	0.0000	1.0
Eu 2	0.9971	0.2500	0.2500	0.6667
Na1	0.9971	0.2500	0.2500	0.3333
Mo1	0.0000	0.7500	0.2500	1.0
O1	0.3482	0.1029	0.9094	0.9166
O2	0.1641	0.1641	0.1641	1.0
F1	0.3482	0.1029	0.9094	0.0834

Table S3. Equivalent circuit fit parameters for the complex impedance plots of the oxidized NSMF and NEMF samples in a dry air and dry Ar atmosphere at 500 °C.

Sample	*R*, Ohm×10^6	*CPE*, T×10^{-11}	*CPE*, P
NSMF (dry air)	0.11±0.01	1.78±0.02	0.95±0.01
NSMF (dry Ar, pO_2 = 0.002 atm)	0.11±0.01	2.27±0.02	0.93±0.01
NEMF (dry air)	0.19±0.01	2.71±0.02	0.92±0.01
NEMF (dry Ar, pO_2 = 0.055 atm)	0.18±0.01	2.59±0.02	0.92±0.01
NEMF (dry Ar, pO_2 = 0.011 atm)	0.18±0.01	2.60±0.02	0.93±0.01
NEMF (dry Ar, pO_2 = 0.002 atm)	0.19±0.01	2.48±0.02	0.93±0.01