Ionic Conductivity of Na₃Al₂P₃O₁₂ Glass Electrolytes – Role of Charge Compensators

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Sample	Na	Al	Р	Si	Ο	Total
						Atoms
Si0	450	300	450	0	1800	3000
Si50	488	326	424	481	1955	3274
Si100	456	306	334	152	1826	3074
Si150	428	286	258	214	1716	2902

Table S1: The number of atoms used for the simulation of glasses

Table S2: Cut-off radii used to compute the nearest neighbours

Sample	Cut-off radii (A)
Si-O	2.00
Na-O	3.15
Al-O	2.40
P-O	2.20



Figure S1: Total percentage of Na connected to BO and NBO as a function of SiO₂ (mol%).



Figure S2: Equivalent circuit models used for the fitting of (a) single semi-circle and (b) two semi-circles impedance spectra.



Figure S3: The surface meshes showing the network (blue) and modifier rich channel (red) regions of Si0 (figure a, c & e) and Si150 (figure b, d & f) glass samples obtained from the MD simulations.



Figure S4: The atomic arrangement of Na and its neighbours in Si0 and Si150 glass sample. The Na surrounded by five P—NBO bonds in the modifier rich channel region of NAP glass, and Na surrounded by two P—NBO and three BO bonds at the interface of modifier rich channel region and network region in NAPS150 glass.