Supporting Information: Atomic-scale investigation of cation doping and defect clustering in the anti-perovskite Na₃OCl sodium-ion conductor

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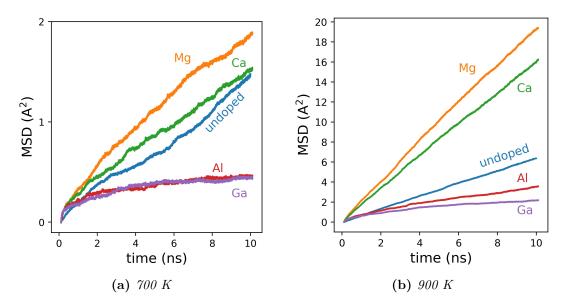


Figure S1: Representative examples of mean square displacement data for undoped (0.1% vacancy concentration) and cation doped (1.2% vacancy concentration) Na_3OCl at two temperatures. Note different y-axis scales.

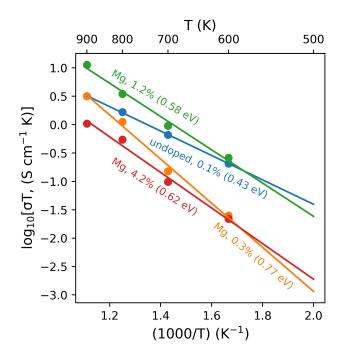


Figure S2: Temperature-dependent Na^+ conductivities (σT) for Mg-doped Na_3OCl at three sodium vacancy concentrations compared to the undoped system. 4.2% Mg-doping shows lower ionic conductivity than the 1.2% level.