

Abstract Submitted
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Computational study of Li₂OHCl as a possible solid state battery material¹ JASON HOWARD, N. A. W. HOLZWARTH, Wake Forest University — Preparations of Li₂OHCl have recently been experimentally studied^{2,3} as solid state Li ion electrolytes. A disordered cubic phase is known⁴ to be stable at temperatures $T > 35^\circ$ C. Following previous ideas,³ first principles supercells are constructed with up to 320 atoms to model the cubic phase. First principles molecular dynamics simulations of the cubic phase show Li ion diffusion occurring on the $t = 10^{-12}$ s time scale, at temperatures as low as $T = 400$ K. The structure of the lower temperature phase ($T < 35^\circ$ C) is not known in detail⁴. A reasonable model of this structure is developed by using the tetragonal ideal structure found by first principles simulations and a model Hamiltonian to account for alternative orientations of the OH groups. ² Hood *et al.* **JACS** **138**, 1768-1771 (2016). ³ Li *et al.* **Angew. Chem. Int. Ed.** **55**, 9965-9968 (2016). ⁴ Schwering *et al.* **CHEMPHYCHEM** **4**, 343-348 (2003).

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