

## Electronic Supplementary Information (ESI)

### An Efficient Rule-Based Screening Approach for Discovering Fast Lithium Ion Conductors Using Density Functional Theory and Artificial Neural Networks

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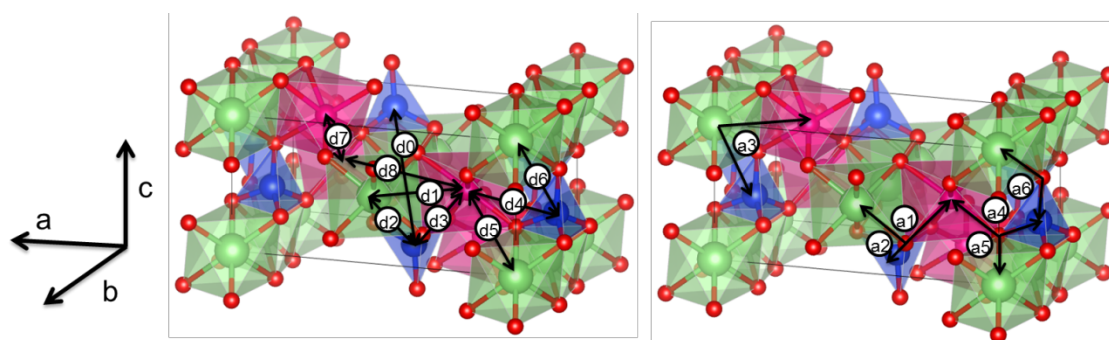


Figure S1. Illustration of the inter-polyhedron parameters within the unit cell that are used as input variables. The description and variable code assignment is shown in Table 1 of the main text.

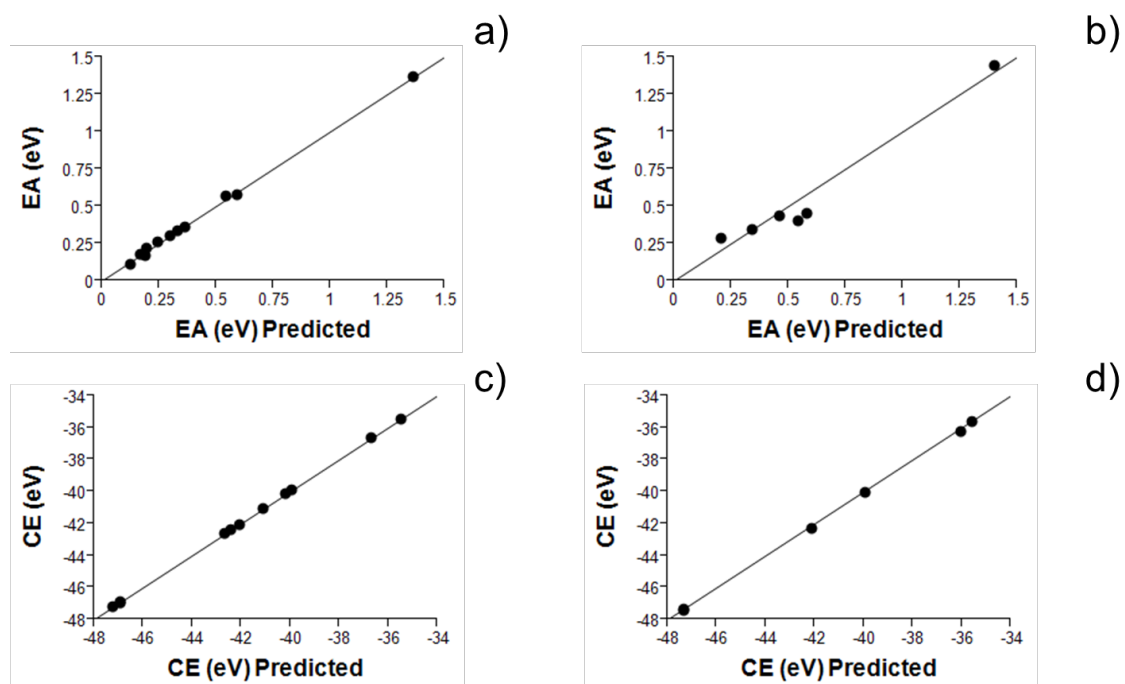


Figure S2. Fitting quality related to a)-c) training and b)-d) validation steps for the chosen final literature-driven NN model (LN3) with simultaneously fitted EA and CE values. The straight line represents the ideal fit.

