High-throughput computational screening of fast Li-ion conductors

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1. Broader Context

I. Motivation
- Conventional electrolytes are volatile and flammable.
- Solid State Electrolytes (SSE) have higher energy density and high operable temperature.

II. Problem
- Experimental approaches for materials discovery is human intensive and not easily scalable, hence the need for computational screening.
- To compute ionic conductivity on hundreds of structures a fast and accurate potential is required.

III. Method
- AiiDA serves as an infrastructure to automate and manage the complex workflows required in this screening [1] [2]. An example provenance -

2. Results

I. Overall screening workflow

II. Bandgap study

Fig. 2 Geometry optimisation is not strictly necessary as (a) for most structures neither volume nor bandgap changes significantly on relaxation, (b) and very few (~5%) structures were misidentified as conductors (false +ve) or insulators (false –ve), if not released

3. Conclusions

With this workflow implemented in AiiDA, one can find fast Li-ion conductors making use of the pinball model to run MD calculations that are as precise as ab initio MD while being a few hundred times less computationally expensive.

4. References

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