SUBLIME

Solid state sUlfide Based LI-MEtal batteries for EV applications

Deliverable 7.1 Properties prediction of sulfide solid electrolyte

Javier Carrasco
CIC energiGUNE

Andrey Golov
CIC energiGUNE

Sublime is funded by the European Union's H2020 research and innovation programme under GA Agreement no. 875028

Publishable summary

Work Package 7 of SUBLIME project focuses on driving the iterative development of SUBLIME material and cell sulfide solid-state battery technology through physics-based multiscale modelling. In this first report, we present the outcome of atomistic simulations devoted to predicting key properties of the sulfide solid electrolyte. Specifically, the interfacial geometries, reactivity, and Li-ion conductivity of the electrolyte at bare and coated Li-metal anodes were evaluated based on ab initio molecular dynamics simulations combined with a novel topological analysis of procrystal electron densities. This deliverable also includes an account of the impact of humidity on the cell characteristics and safety aspects, as predicted from the thermodynamics of the electrolyte hydrolysis computed with density functional theory calculations. Main conclusions are summarized at the end of this document.