Simulating transport properties of solid-state electrolytes via machine-learning models

Monday July 24th, 2023 – 11.00 (sharp)
Room L1.3, 1st Floor, Physics building
Remote link: Teams

Speaker
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Abstract
Transport phenomena, like heat and charge conduction, are of paramount importance in materials science and technology, as they govern the efficiency of devices, fuel cells, and heat exchangers. Specifically, in the current quest for solid-state electrolytes (SSE) for the next generation of batteries, a tradeoff between a high flow of ionic charge - crucial for fast charging and large power needs - and a fast heat dissipation must be found to avoid overheating or explosions. In my talk, I will show how modelling transport phenomena in SSE strongly benefitted, in the last few years, from substantial theoretical advancements on the fundamentals of ab-initio heat and charge transport [1,2], as well as from machine-learning force fields, reaching ab-initio accuracy in the description of interatomic interactions, while keeping a linear scaling with system size [3]. I will showcase these approaches on typical SSE of particular interest thanks to the non-toxicity and large availability of their constituents, namely lithium chlorates and lithium thiophosphates [3,4]. I will conclude by commenting on finite-size effects in the ionic dynamics and thermal transport of superionic conductors [5], and by illustrating recent results on the robustness of the predictions of ML models [6].

References:

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