UNIMORE Dipartimento di Scienze Fisiche, Informatiche e Matematiche
UNIVERSITÀ DEGLI STUDI DI MODENA E REGGIO EMILIA

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FIM-S3 SEMINAR

Invariance principles of transport coefficients and their application to superionic conductors

Friday July 8th, 2022 – 11.00

S3 Seminar Room, 3rd floor, Physics building

Speaker

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Abstract

The Green-Kubo theory of linear response makes it possible to extract transport coefficients, like diffusion coefficients or the electric and thermal conductivities of a material, from the time correlation functions of properly defined fluxes that can be sampled via equilibrium molecular dynamics simulations [1]. In my talk I will start by summarizing some recent advances on this topic. In particular, I will discuss some invariance principles according to which the transport coefficients are largely independent of the definitions of atomic quantities [2,3]. I will then show how to obtain accurate estimates of the thermal conductivity and its uncertainty from relatively short trajectories, thanks to the multivariate cepstral analysis of the time series of the fluxes involved in transport processes [4,5]. I will showcase these theoretical and data analysis tools for the paradigmatic examples of superionic water [6] and a typical Li-ion solid-state conductor, Li_3ClO [7]. I shall conclude with a thorough investigation of finite-size effects in the ionic dynamics and thermal transport of superionic conductors [8].

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[4] Ercole, L., Marcolongo, A., & Baroni, S. (2017). Accurate thermal conductivities from optimally short molecular dynamics simulations. Scientific reports, 7(1), 1-11.
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[8] Grasselli, F. (2022). Investigating finite-size effects in molecular dynamics simulations of ion diffusion, heat transport, and thermal motion in superionic materials. The Journal of Chemical Physics, 156(13), 134705.

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