

FIM-S3 SEMINAR

Spectral methods for the analysis of transport phenomena in electronic insulators

Monday July 7th, 2025 – 10.00 (sharp)

Room L1.3, 1st Floor, Physics building

Remote link: [Teams](#)

Speaker

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Abstract

Understanding and controlling heat and charge transport is central to the design of efficient thermoelectric materials and solid-state ionic conductors. However, the prediction of transport coefficients from equilibrium molecular dynamics remains challenging, requiring long simulations and robust statistical tools. I will present a unified framework based on spectral analysis of current time series, enabling the accurate computation of the full Onsager matrix—including both diagonal and off-diagonal transport coefficients—from a single statistical model. The method is demonstrated on molten salts, liquid water, and the Li_3PS_4 solid-state electrolyte. Building on this, I will explore the microscopic origins of thermal transport in the Li_3ClO antiperovskite, where a combination of ab initio, machine-learning, and empirical force-field simulations reveals the key roles of anharmonicity and ionic diffusion in characterizing thermal conductivity. Finally, I will briefly turn to the case of SiGe thermoelectrics, showing how spatially correlated mass disorder can strongly suppress lattice heat transport and provide a viable pathway to enhancing thermoelectric performance through engineered disorder.

Host: Federico Grasselli

In collaboration with

