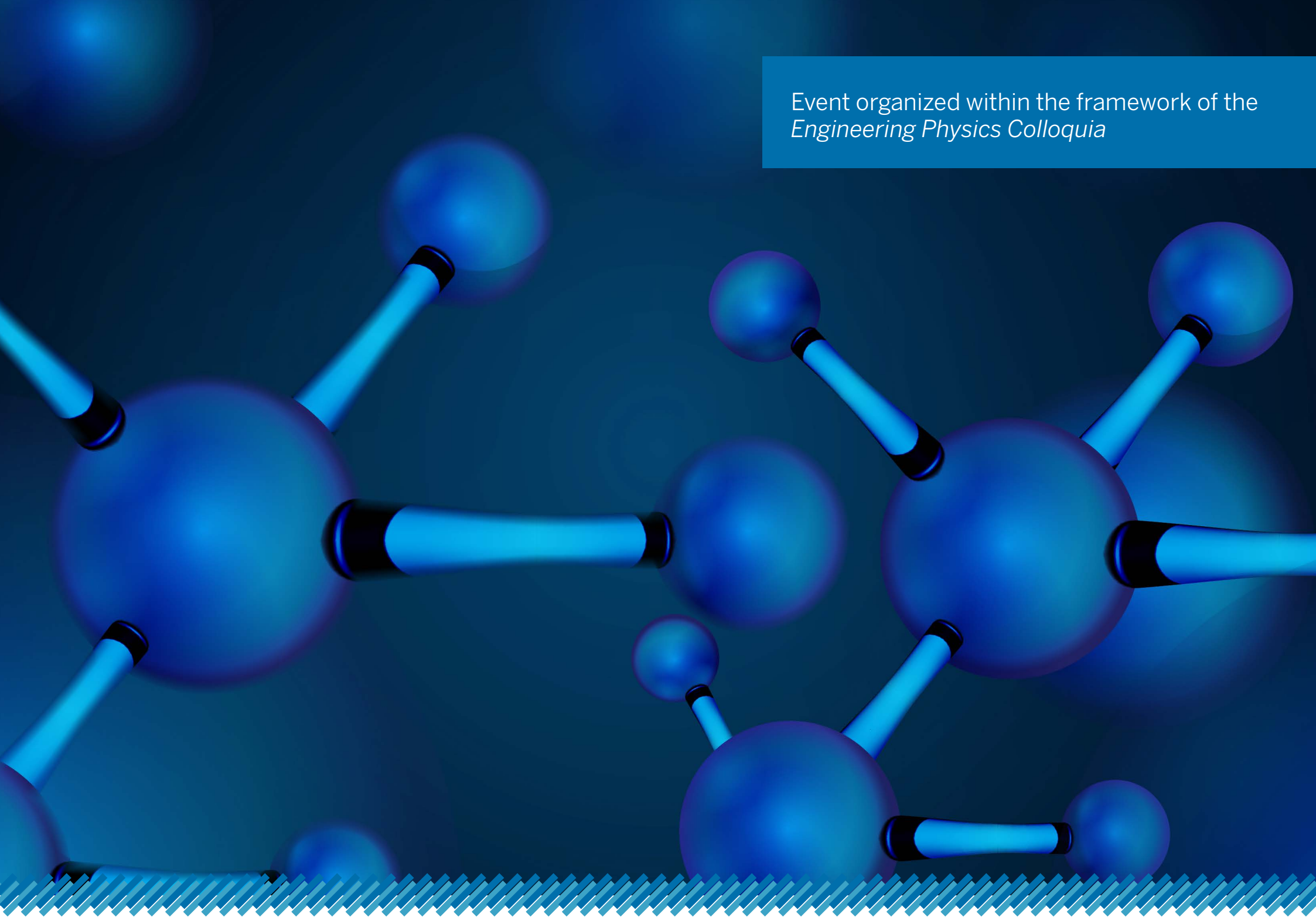

Event organized within the framework of the *Engineering Physics Colloquia*


Ca' Foscari University of Venice

**Department of Molecular Sciences and Nanosystems**

Prof. **Alessandro Laio**
SISSA (Italy)


# *Inferring causality in time-reversible molecular dynamics*

**21st May 2026, 12.00**
Conference Room Orio Zanetto, Alfa Building

The seminar will also be accessible remotely via the following link:**https://unive.zoom.us/j/88538819345**
Password: seminar1

Organized by
**Domenico De Fazio**
**Achille Giacometti**


The ability to distinguish between correlation and causation of variables in complex systems remains an interesting and open area of investigation. In this lecture, we will discuss how causality can emerge in systems evolving according to a time-reversible dynamics and satisfying detailed balance, such as a molecular system simulated by molecular dynamics. We will first introduce the traditional approach to infer the presence of a putative causal link in time series, based on the estimate of the transfer entropy. We will then discuss how this approach can be extended to build a causal graph, synthesising causal relationships between many variables. Finally, we will discuss how one can computationally verify if a putative causal link, corresponding to a strongly asymmetric information transfer between two variables, corresponds to a genuine causal link, or is instead an artifact determined by an unobserved variable that causes the two observed variables.