UNIVERSITÀ DI TRENTO
Dipartimento di Fisica

Dr. Mikko Karttunen

Dept. of Technical Physics, University of Eastern Finland, Kuopio, Finland

ELLIS (European Laboratory for Learning and Intelligent Systems) Institute Finland, Espoo, Finland

January 21, 2026
Room A110

Machine learning in structural analysis of biological soft matter

Abstract

In this talk, I will give a brief overview of structural characterization of soft matter using machine learning. I will discuss two specific examples: 1) molecular level conformational analysis [1], and 2) atomic level characterization of units such as side chains in polymers [2]. The former is particularly relevant for systems undergoing phase transitions while the latter can be used for improvement of force fields, and the latter yields molecular level information that can additionally be helpful in force field development.

[1] Elucidating Lipid Conformations in the Ripple Phase: Machine Learning Reveals Four Lipid Populations. Davies, Matthew; Reyes-Figueroa, A. D.; Gurtovenko, Andrey A.; Frankel, Daniel; Karttunen, Mikko.

Biophys. J. 122, P442-450 (2023).

[2] Learning glass transition temperatures via dimensionality reduction with data from computer simulations: Polymers as the pilot case. Glova, Artem; Karttunen, Mikko. J. Chem. Phys. 161, 184902 (2024).

Contacts:

Staff di Dipartimento di Fisica

0461 28-1504-1575-2042-1545

df.supportstaff@unitn.it

Contatti referenti

prof. Gianluca Lattanzi