Seminar/Talk

ELLIS Talk - Advancing molecular simulation with machine learning

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Host: Bingqing Cheng

Molecular simulation may ideally serve as a "computational laboratory", with is ability to observe both structure and dynamics at high resolution and to simulate molecules that are difficult to synthesize. However, it also suffers from fundamental limitations, in particular in the accurate modeling of molecules and in the efficient computation of experimental observables. By leveraging the latest developments in machine learning, we can advance molecular simulation algorithms to make significant progress at these fronts without sacrificing rigorous physics.In this talk, I will give an overview over our work on the highly accurate computation of quantum states with deep fermionic neural networks and Quantum Monte Carlo, and addressing the many-body sampling problem using deep Markov State Models and generative deep learning.

Monday, May 9, 2022 02:00pm - 04:00pm
Raiffeisen Lecture Hall, Central Building

This invitation is valid as a ticket for the ISTA Shuttle from and to Heiligenstadt Station. Please find a schedule of the ISTA Shuttle on our webpage: https://ista.ac.at/en/campus/how-to-get-here/ The ISTA Shuttle bus is marked ISTA Shuttle (#142) and has the Institute Logo printed on the side.