CONDENSED MATTER COLLOQUIUM SERIES

#Ankara

Emine Küçükbenli

NVIDIA

Generative AI for drug discovery and materials science

Generative Artificial Intelligence is transforming drug discovery and materials science by enabling the design of novel molecules and converting traditional simulation tasks into generative processes. In drug discovery, AI is accelerating the development of new drug candidates by generating molecules optimized for specific properties, increasing their potential to become effective therapeutic agents. In materials science, machine-learned interatomic potentials are improving the efficiency and accuracy of simulations, providing deeper insights into molecular and material behavior at the atomic scale. Both fields are benefiting from AI's ability to speed up traditionally computationally expensive and time-consuming simulations that are crucial for predictive modeling. This talk will explore the latest advancements in AI-driven drug and material discovery, highlight the role of generative methods in accelerating simulations, and discuss the challenges and future directions required to scale these innovations for industrial applications.

January, 14, 2025
Tuesday

19:00, (Ankara Time)

Click here for zoom link
Meeting ID: 432 931 6595
Password: 326852

Emine Küçükbenli is a Research Manager at NVIDIA since 2022, leading research and product development efforts within BioNeMo, NVIDIA's AI-based drug discovery platform, as well as cuEquivariance, a GPU accelerated math library for symmetry aware neural networks. Before NVIDIA, Emine was a faculty at Information Systems Dept, Boston University, and before that, postdoctoral researcher at Harvard School of Engineering and Applied Sciences and Ecole Polytechnique Federal de Lausanne. Emine got their PhD from SISSA, Italy in computational condensed matter physics, and is deeply grateful to state-of-the-art undergraduate education they received in Physics at Bilkent University, Turkey.
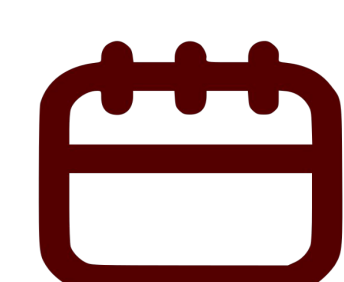
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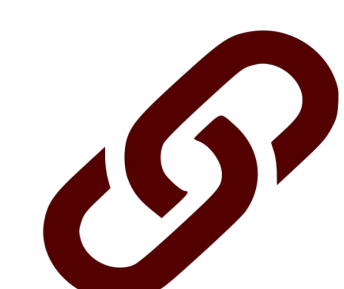If you'd like to sign up to the mailing list to receive announcements and remainder, please use:
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