CONDENSED MATTER COLLOQUIUM SERIES

#Ankara

Deniz Günceler

Microsoft Research AI4Science

Transformation of natural sciences through large-scale AI & Machine Learning

Application of large machine learning models, in particular large language models, is transforming the global economy. Likewise the natural sciences have also benefited from these new developments, with generative models such as MatterGen or Gnome transforming how we discover new materials. This talk will focus on Skala, a recently published machine-learned exchange correlation (XC) functional for density functional theory (DFT) constructed using deep learning. We show that XC functionals can be learned from more accurate quantum chemical data, such as Couple Cluster and Quantum Monte Carlo. Skala represents a major advancement in the field of density functional theory by achieving accuracy competitive with (or better than) the best-performing hybrid functionals, at the much lower computational cost of semi-local DFT. More importantly Skala demonstrates the possibility of constructing more accurate and faster DFT methods by scaling up training data.

Sep, 16, 2025
Tuesday

19:00, (Ankara Time)

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

Deniz Günceler is a Principal Research Engineering Manager at Microsoft Research AI4Science. After receiving his BS from Bilkent University, he earned his PhD in physics from Cornell University. Following 8 years working at Amazon Alexa GenAI, he joined Microsoft Research in 2023. His research interests lie at the intersection of machine learning and computational science.

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