



Department of Materials Science
& Engineering
College of Design and Engineering

Department Seminar

Extending semiconductor device simulations to complex materials

Date: 02 July 2026

Time: 3:00 PM – 4:00 PM

Venue: EA LT7, Level 1



Manasa Kaniselvan

Incoming Assistant Professor at MIT
PhD candidate, ETH Zurich, Switzerland

Abstract

Semiconductor devices are now approaching atomic-scale miniaturization, making it both possible and increasingly necessary to design them at atomistic resolution. To do this, we need to combine a materials-level description of different device components with the physics of non-equilibrium quantum transport under voltage bias. The link between these two computational frameworks is the electronic structure, typically given by the Hamiltonian matrix in the atomic orbital basis. Here, I will present recent work on developing Machine Learned (ML) property models to generate Hamiltonian matrices rapidly, for arbitrary materials, and at large scales, enabling downstream transport simulations of entire devices. I will review methods in (1) data handling, (2) architectural setup, and (3) computational deployment, which together allow for training on terabyte-scale Hamiltonian matrix datasets and inference on structures with several thousands of atoms. Finally, I will present how scalable ML electronic structure models can unlock the ability to tackle new design problems for semiconductor materials.

Biography

Manasa Kaniselvan is a PhD candidate in the Computational Nanoelectronics Group at ETH Zurich, Switzerland. Her research aims to bring atomistic and *ab initio* materials simulations to the scale of semiconductor devices by leveraging machine-learned (ML) materials foundation models, advanced transport codes, and scalable custom applications. She has previously worked with teams at Samsung Semiconductor and Meta FAIR (Fundamental AI Research) Chemistry, where she contributed towards the development of semiconductor device/process simulations and designed scalable ML electronic property models. In 2027, she will join the faculty at MIT as a tenure-track assistant professor, jointly in the departments of Materials Science and Engineering (DMSE) and Electrical Engineering and Computer Science (EECS) through a Schwarzman College of Computing shared position.

Looking forward to seeing all of you!

Hosted by: Peichen Zhong