# Houk-Jung Organic Colloquium

## Synthesis and Catalysis with Predictive Analytics

**Abstract:** The synthesis of natural products is motivated by their potent biological effects, enigmatic biosynthetic origins, and complex molecular structures. Computational tools such as density functional theory and machine learning can provide mechanistic insights and predict reactivity in silico to inform synthetic campaigns. In addition, computational tools and predictive analytics can guide the development and application of transition-metal catalysis. Several examples of computational approaches to challenges in synthesis and catalysis are presented: selectivity rationalization during the synthesis of berkeleyone A, machine learning to guide the synthesis of clovane terpenoids, hybrid modeling to predict the site of late-stage functionalization of pharmaceutical intermediates, and machine learning to develop new catalysts for olefin hydroformylation. These advances enable more efficient use of synthetic resources and offer modern solutions to pressing challenges in synthesis and catalysis.

**Bio:** Masha was born in Moscow, Russia and grew up outside of Boston, Massachusetts. She completed her BA in Chemistry at Washington University in St. Louis in 2014, working with Prof. Vladimir Birman on the development of amidine-based ligands for asymmetric catalysis. She completed her Ph.D. in 2019 at Yale University in the group of Prof. Timothy Newhouse. In the Newhouse group, her research included the synthesis of meroterpenoid natural products, the study of biomimetic terpene rearrangements, and the development of computational tools for natural products synthesis. In January of 2020, Masha moved to work with John Hartwig at UC Berkeley as an NIH Postdoctoral Fellow, where her research focuses on developing computational approaches to predict the selectivity of transition-metal catalyzed reactions, including arene borylation and olefin hydroformylation.

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**Thursday, Jan 12, 2023 | 4:00 PM**
**Mani L. Bhaumik Collaboratory - YH 4222**
**Dongwon Yoo Seminar & Conference Hall**

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