

Physical Chemistry Seminar

Mutexa: A Physics-based Ecosystem for Intelligent Protein Engineering

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Protein engineering creates functional proteins and variants that suit our needs for synthesis, therapeutics, and sustainability. Despite the success of directed evolution, protein engineering stumbles when its protein targets fail to work with high-throughput screening. My vision is to create Mutexa, a molecular modeling-informed ecosystem that allows researchers to seamlessly acquire sequences of proteins and variants with desired functions as biocatalysts and therapeutic peptides, akin to Amazon Alexa's role as a virtual assistant. In this talk, I will present the technical foundations of Mutexa and its application in two protein engineering challenges: one for designing industrial bidomain enzymes that maintain high activity at lower temperatures (known as cold-adapted enzymes), and the other for predicting the structures of lasso peptides, a class of ribosomally synthesized and post-translationally modified peptides (RiPPs) as antibiotics. These applications showcase Mutexa's unique ability to drive the discovery of functional proteins beyond traditional screening-based approaches, offering solutions for sustainable biomanufacturing and antimicrobial development.



Wednesday, February 12, 2025



10:30am



BRWN 4102



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Yang Bio

Zhongyue John Yang is the SC Family Dean's Faculty Fellow, Assistant Professor of Chemistry, Chemical and Biomolecular Engineering at Vanderbilt University. He graduated from the inaugural Chemistry Po-Ling class at Nankai University in 2013, earned his Ph.D. in Theoretical and Computational Chemistry with Ken Houk at UCLA in 2017, and undertook postdoctoral training with Heather Kulik in the Department of Chemical Engineering at MIT from 2018 to 2020. Since fall 2020, he has started his independent research group at Vanderbilt. His research emphasizes establishing "Mutexa", a virtual platform aiming to revolutionize protein engineering, envisioning a future where creating beneficial protein variants is as effortless as using Amazon Alexa. He is a recipient of NIH Maximizing Investigators' Research Award in 2022, Robin Hochstrasser Young Investigator Award in 2023, and ACS OpenEye Junior Faculty Award in Computational Chemistry in 2024. He is a member of the Early Career Board for the Journal of Chemical Theory and Computation by the ACS Publications.