Zernike Colloquium

January 12th, 2023
16:00h
BB 5161.0105

Inverse Molecular Design for Organic Electronic Materials and Catalysts

by Robert Pollice

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Inverse molecular design starts at the desired properties and explores the chemical space to identify molecules optimizing them. In recent years, advances in machine learning combined with high-throughput virtual screening have revolutionized inverse design and made it readily applicable to a wide range of problems. In this talk, I will demonstrate how simple representations of molecules can give rise to powerful inverse design algorithms that can be applied for designing promising organic light-emitting diode materials. In my outlook, I will talk about how we will use these techniques together with lab automation to tackle problems in homogeneous catalysis.

Coffee from 15:30h
Drinks & Snacks after

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