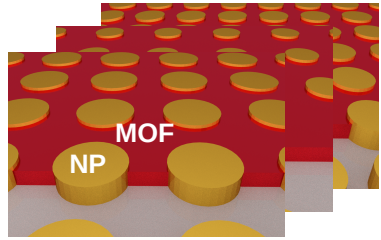


Inverse Design of Nanoparticle Metal-Organic Framework

Graduate Student Fellows: Jingtian Hu, Tom Zhao Faculty Advisers: Teri Odom, Neelesh Patankar

Research Objective: We propose a design cycle for coupled NP/MOF structures that optimizes the system geometry and materials selection for tasks such as gas storage, drug delivery and catalysis.

Optimization Scheme

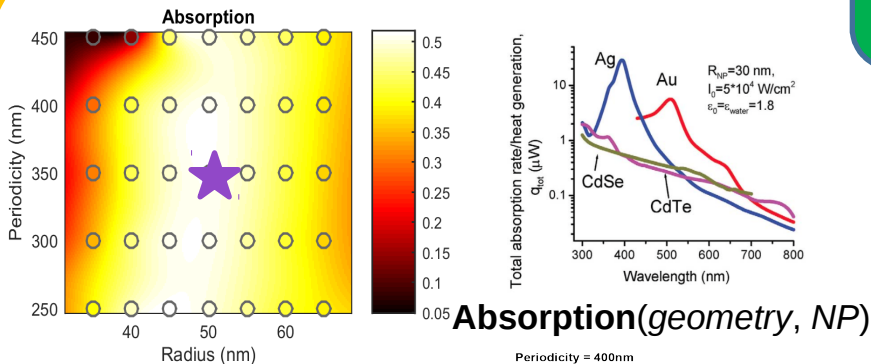


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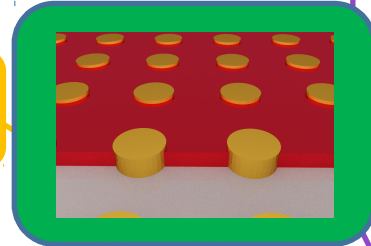
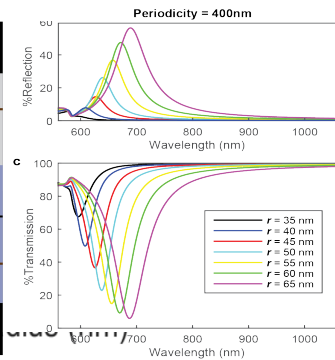
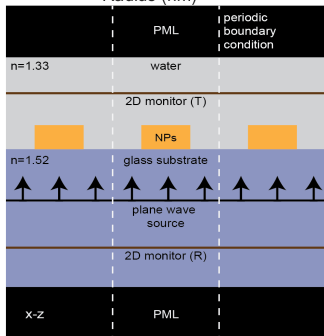
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NP, MOF, geometry

Optical Absorption

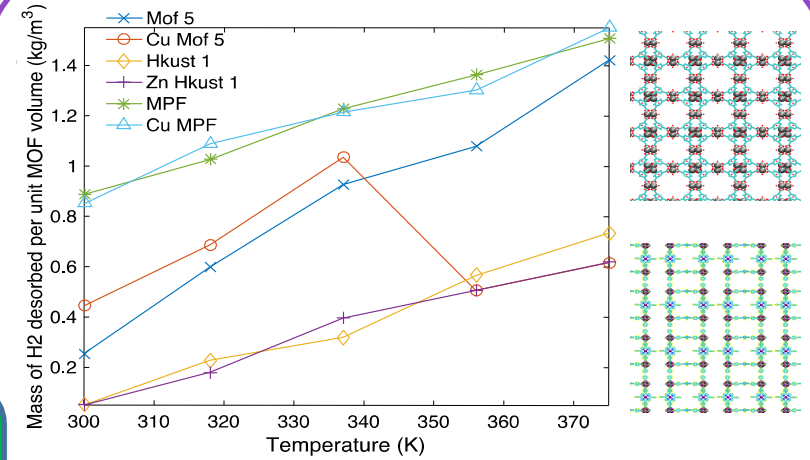


Absorption(geometry, NP)



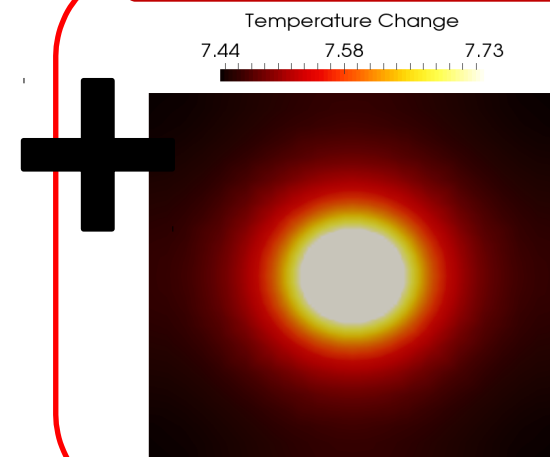
Optimized Structure

MOF Reactions



Gas Storage (geometry, MOF)

Temperature Field



Temperature(x,y,z)