



Contribution ID: 174

Type: **Talk**

Insights into the nature of host-guest interactions in emergent framework materials

Monday, 14 March 2022 15:50 (20 minutes)

We use various computational methods (DFT, molecular docking, interaction analysis) to characterize and quantify the host-guest interactions in metal-organic and covalent organic frameworks. We will show results for several different application cases and discuss their relation to experimental findings.

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Session Classification: Theory

Track Classification: Main conference: Engineering Materials and Applications