

Invitation for the Webinar

"Importance of Catalysis, AI, and Data for EHLCATHOL"

Thursday, February 22, 2024

01:00 p.m. Welcome

Prof. Matthias Beller; LIKAT, Prof. Yongdan Li, Aalto University

01:10 p.m. "Machine Learning Strategies for Secondary Sphere Modification in

Organocatalysis"

Prof. Anat Milo, Ben-Gurion University of the Negev, Israel

02:00 p.m. "National Data Infrastructure for Catalysis (NFDI4Cat)"

Dr. David Linke, LIKAT

02:40 p.m. "New AI based software for the RON estimation of EHLCATHOL

biofuels."

Roda Bounaceur, CNRS - LRGP

03:10 p.m. "Artificial intelligence-assisted exploration of lignin solvolysis

mechanisms: speeding up molecular dynamics simulations based

on density functional theory"

Gen Li, Aalto

03.40 p.m. Conclusion and closing

Prof. Matthias Beller; LIKAT, **Prof. Yongdan Li**, Aalto University

Join Zoom-Meeting

https://uni-rostock-de.zoom-x.de/j/62392371217?pwd=V0IrdjhMWDZiQ0pUb1lzM2IFd09vdz09



