

BiGmax Workshop 2021

Wednesday, 14 April 2021

Session I: Computational material synthesis (Chair: Peter Fratzl) (13:45 - 15:30)

time	[id] title	presenter
13:45	[54] Computational material synthesis: Atomistic and molecular dynamics, and bio-inspired AI (30 min talk + 15 min discussion)	BUEHLER (INVITED), Markus
14:30	[39] AI-driven discovery of material "genes": application to CO ₂ activation on semiconductor oxide surfaces (12 min talk + 3 min discussion)	GHIRINGHELLI, Luca
14:45	[50] Design of high-entropy Invar alloys via machine learning (12 min talk + 3 min discussion)	RAO, Ziyuan
15:00	[43] Data-driven search for drug–membrane permeability models (12 min talk + 3 min discussion)	DUTTA, Arghya
15:15	[51] Data driven approaches to design damage tolerant Dual-phase steel microstructures (12 min talk + 3 min discussion)	KUSAMPUDI, Navyanth