Accelerated Discovery of New Materials

787. WE-Heraeus-Seminar

15 – 18 May 2023

at the Physikzentrum Bad Honnef, Germany

WILHELM UND ELSE HERAEUS-STIFTUNG

Program

Monday, 15 May 2023

11:00 – 15:00	Registration	
12:30 – 13:45	*LUNCH*	
14:00 – 14:15	Scientific organizers	**Opening remarks**
14:15 – 15:00	Claudia Draxl	**The FAIRmat approach to accelerated discovery of new materials**
15:00 – 15:30	*COFFEE BREAK*	
15:30 – 16:15	Pascal Friederich	**Machine learning for simulation, understanding and design of molecules and materials**
16:15 – 17:00	Jonathan Schmidt	**Machine learning discovery of materials**
17:00 – 17:45	Manuel Tsotsalas	**Accelerated MOF synthesis via automated data extraction and machine learning**
18:30 – 20:00	*DINNER*	
20:00 – 20:45	Berend Smit	**Big data in chemistry and chemical engineering: Science beyond understanding**
20:45 – 21:00	Hartmut Gliemann	**Present status and future of fully automated production and application of surface-anchored metal-organic framework (SURMOF) based coatings at IFG – an overview**
21:00 – 21:15	Dinga Wonanke	**A step towards predicting synthesis conditions of metal-organic frameworks**
21:15 – 21:30	Qiang Zhang	**Exploring the Mechanical Properties of a 2D MOF: A Combined MD Simulation and Experimental Study**

Program

Tuesday, 16 May 2023

08:00	*BREAKFAST*	
09:00 – 09:45	Larry Lüer	**Autonomous discovery of semiconducting materials for photovoltaics**
09:45 – 10:30	Seda Keskin	**Computational modeling of MOFs for gas separations**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Regine Willumeit-Römer	**Towards a digital twin for degradable Mg-implants**
11:45 – 12:30	Ziyuan Rao	**Machine learning-enabled high-entropy Invar alloy discovery**
12:30– 12:40	**Conference Photo** (in the front of the lecture hall)	
12:40 – 14:00	*LUNCH*	

Program

Tuesday, 16 May 2023

14:00 – 14:15	Anna Kornyushchenko	**Formation of porous metal nanosystems under near-equilibrium condensation conditions in plasma-condensate system**
14:15 – 14:30	Tomasz Ossowski	**Superconductivity in high entropy alloys**
14:30 – 14:45	Andreas Terfort	**Parallel electrochemical investigation of combinatorial catalytic system**
14:45 – 15:30	**Poster Flash 1** *(poster presenters will be announced)*	
15:30 – 16:00	*COFFEE BREAK*	
16:00 – 18:00	**Poster session 1**	
18:30 – 20:00	*DINNER*	
20:00 – 20:45	Giorgio Sangiovanni	**Dirac fermions on the triangular lattice**
20:45 – 21:00	Brian Richard Pauw	**Synthesizing a library of 1000+ reproducible MOFs**

Program

Wednesday 17 May 2023

08:00	*BREAKFAST*	
09:00 – 09:15	Roland A Fischer	**Structure-activity relationships in metal-organic frameworks' conversion for Oxygen evolution reaction**
09:15 – 10:00	**Poster flash 2** *(poster presenters will be announced)*	
10:00 – 10:30	*COFFEE BREAK*	
10:30 – 12:30	**Poster session 2**	
12:30 – 14:00	*LUNCH*	
14:00 – 17:00	**Excursion**	
18:30	*HERAEUS DINNER* *(social event with cold & warm buffet with complimentary drinks)*	

Program

Thursday, 18 May 2023

08:00	*BREAKFAST*	
09:00 – 09:45	Helge Stein	**Progress, prospects and the future of autonomous chemistry**
09:45 – 10:30	Axel Groß	**The use of descriptors in the accelerated discovery of battery materials with improved properties**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Wolfgang Wenzel	**Virtual materials design**
11:45 – 12:30	Scientific organizers	**Poster prize and closing remarks**
12:30	*LUNCH*	

End of the seminar and departure

NO DINNER for participants leaving on Friday; however, a self-service breakfast will be provided on Friday morning