COST workshop Catalytic water splitting

Date: Tuesday September 21st -
Wednesday September 22nd 2021
Location: ZOOM

Tuesday September 21st

9:30-9:35	Opening	
9:35-10:15	The potential of abundant metals for catalyzing the water dissociation reaction	José R. B. Gomes
10:15-10:55	Constant inner potential DFT - a general method for constant potential DFT calculations.	Marko M. Melander
10:55-11:10	Break	
11:10-11:50	Rational Design of Semiconductor Interfaces for Photocatalysis	Giovanni Di Liberto
11:50-12:15	Mixing ReaxFF parameters for transition metal oxides using force-matching method.	Bartek Szyja
12:00-13:30	Lunchbreak	
13:30-14:30	MC Meeting	
14:30-15:30	Discussion: Restarting the Action after COVID19	

Wednesday September 22nd

9:30-9:55	Enzyme-sulphide coupling for light-induced water splitting	José C. Conessa
9:55-10:35	Evolution of step edges on catalytic surfaces	Magdalena Załuska-Kotur
10:35-10:50	Break	
10:50-11:15	Computational modelling of ceria-supported platinum catalysts under reactive conditions: Global optimization and ab initio thermodynamics study	Jon E. Quinlivan
11:15-11:40	DFT investigation of U3O8//Fe2O3 heterostructures as photoanodes for water splitting.	Leonhard Mayrhofer
11:45-12:10	Using Embedding for Multiscaling - an overview	Florian Libisch
12:10-12:15	Closing	