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17th EC2/BIG-NSE Workshop

Start Time: Friday, January 12, 2024 01:30 pm

End Time: Friday, January 12, 2024 05:00 pm

C264

TU Berlin, Straße des 17. Juni 115, 10623 Berlin, C Building

As every year, once their "initial phase" is finished, the <u>new PhD students</u> of EC²/BIG-NSE have the opportunity to present their PhD work plan in front of the UniSysCat community.

The scope of the presentations ranges from theory to application on all aspects of catalysis: Organic/Inorganic chemistry, heterogeneous catalysis, biotechnologies, biocatalysis etc.: all interested scientists are welcome!

Time	Programme	Lecturer	Superv
13:40-13:50	Welcome words	Maria Andrea	
		Mroginski	
13:50-14:10	Aldehyde oxydase constant of Michaelis prediction using	Daniil Lepikhov	Ariane
	machine learning		Alves,
			Leimkü
			Mrogin
14:10-14:30	Obtaining a dynamic picture of biological carbon fixation by	Denise Poire	Marius
	computational spectroscopy and simulations		Maria N
14:30-14:50	Elucidating coupling and reactivities in an ATPase driven	Zishuo Zhang	Ingo Ze
	reductase complex by vibrational spectroscopy and		Mrogin
	quantum chemical computations		
14:50-15:10	Coffee break		
15:10-15:30	Improved photosystem coupling and a novel spectral-	Laura Mages	Dennis
	tuning approach in light-driven formate production		Athina
			Patrick
15:30-15:50	Structural basis of rhomboid protease substrate recognition	Enlin Zheng	Daniel
	and transmembrane helix arrangement by crvo-FM and		Adam
	integrative modeling		Sun
15:50-16:10	Coffee break		
16:10-16:30	Identification and characterization of halogenases acting on	Jonas Motter	Peter
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	nucleoside scaffolds		Neuba Sun
16:30-16:50	Reductive catalytic fractionation of waste cellulosic- biomass to functional chemicals and subsequently to green polymers	Camila Dias	Majd A Markus Peter N
16:50-17:00	Closing remarks	Maria Andrea Mroginski	

