



Design, implementation and production upscaling of novel, high-performance, cluster-based catalysts for CO₂ hydrogenation

Deliverable D6.3

NWT3: School on electronic structure theory



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First Catchy School: Computational methods for cluster-based (CO₂ conversion) catalysts – April 19-21, 2022, Budapest

The first Catchy school was organized jointly by the Budapest University of Technology and Economics (BME) and Furukawa Electric Institute of Technology Ltd. (FETI). The meeting took place in Budapest, Hungary, and consisted of three days of training (April 19 to 21, 2022) also open to external Master and PhD students and was followed by the midterm review meeting for Catchy members on April 22nd.

The school entitled “Computational methods for cluster-based (CO₂ conversion) catalysts” took place at two different locations: i) the CH Building at BME (on Tuesday and Wednesday 19-20/04/2022) and ii)(on Thursday 21/04/2022) (see full programme below).

The programme contained both S&T training (including an Introduction to computational chemistry and its applications to cluster-based CO₂ conversion catalysis) and broader skills training (including presentations of relevant companies based in Hungary, a training on techno-economical aspects of CO₂ capture and utilization (CCU), an intellectual property training, and a training about the position of women in science). On Thursday morning there was a hands-on workshop to learn how to perform quantum chemical calculations.

A total of 35 participants on Day1, 39 on Day 2 and 26 on Day 3 attended the School in person. There were 12 female participants and 18 external PhD students (one from KU Leuven, the others from the Budapest University of Technology and Economics). The 14 lectures of the S&T and Skills training events were presented by 8 invited speakers outside Catchy network: Tamás Kégl (University of Pécs, HU), Tibor Nagy (Research Center of Natural Sciences, Budapest, HU), Veronika Paksi (TK SZI, Institute for Sociology, Budapest, HU), Attila Wootsch (Mcule.com Ltd), Dávid P. Kovács (University of Cambridge, UK), Alessandro Fortunelli (National Research Council, Pisa, IT), Aleix Comas-Vives (TU Wien, AT) and Orsolya Kéri (Semilab, Budapest, HU) plus 5 speakers from the Catchy partners.







Most of the lectures are made available on the Catchy website for Catchy members.

The School ended with a social dinner and was followed by the Midterm Review on April 22nd that was attended by Catchy’s project Officer Mrs Isabelle Aires Pinto.

The impact of the School was evaluated with an anonymous online feedback form that was sent to all the ESRs and external PhD students that participated to the event. We received 19 feedback forms with an average mark of 7.15/10.

Programme

Time	Description	Presenter	
April 19 (Day 1)	Budapest University, CH Building, Room201	Google Map	
09:00 – 09:45	Arrival/Registration		
10:00 – 10:45	Introduction to Computational Chemistry	Tibor Höltzl University of Budapest, Furukawa EIT, Ltd	
	Coffee / Tea Break		
11:15 – 13:00	Theoretical characterization of transition metal-CO ₂ complexes	Tamás Kégl University of Pécs	
	Lunch		
14:00 – 15:15	Are Experiments Superior over Models?	László Nyulászi University of Budapest	
15:15 – 15:45	Multiphase kinetic modelling of heterogenous catalytic reactions in fixed bed, flow-through reactor systems	Tibor Nagy Research Center of Natural Sciences, Budapest	
	Coffee / Tea Break		
16:15 – 17:15	Women in science, technology, engineering and mathematics (STEM)	Veronika Paksi TK SZI, Institute for Sociology, Budapest	
17:30 – 18:00	Innovation management in practice: Mcule.com Ltd, a successful example	Attila Wootsch Innovation Manager, Mcule.com Ltd	
18:00 – 19:00	Social Program		

April 20 (Day 2)		Budapest University, CH Building, Room201	
09:00 – 10:45	Introduction to Computational Chemistry II	Tibor Höltzl University of Budapest, Furukawa EIT, Ltd	
Coffee / Tea Break			
11:15 – 13:00	Introduction to Machine Learning Interatomic Potentials	Dávid P. Kovács University of Cambridge, UK	
Lunch			
14:00 – 15:55	Theoretical modelling of CO ₂ (electro)reduction catalysis	Alessandro Fortunelli National Research Council, Pisa, IT	
Coffee / Tea Break			
16:25 – 17:25	Atomistic Simulations of the Thermocatalytic Conversion of CO ₂	Aleix Comas-Vives TU Wien, AT AU Barcelona, ES	
17:30 – 18:00	The Semilab Story – From Lab to Fab	Orsolya Kéri	
18:00 – 19:00	Poster session (Coffee / Drinks)		






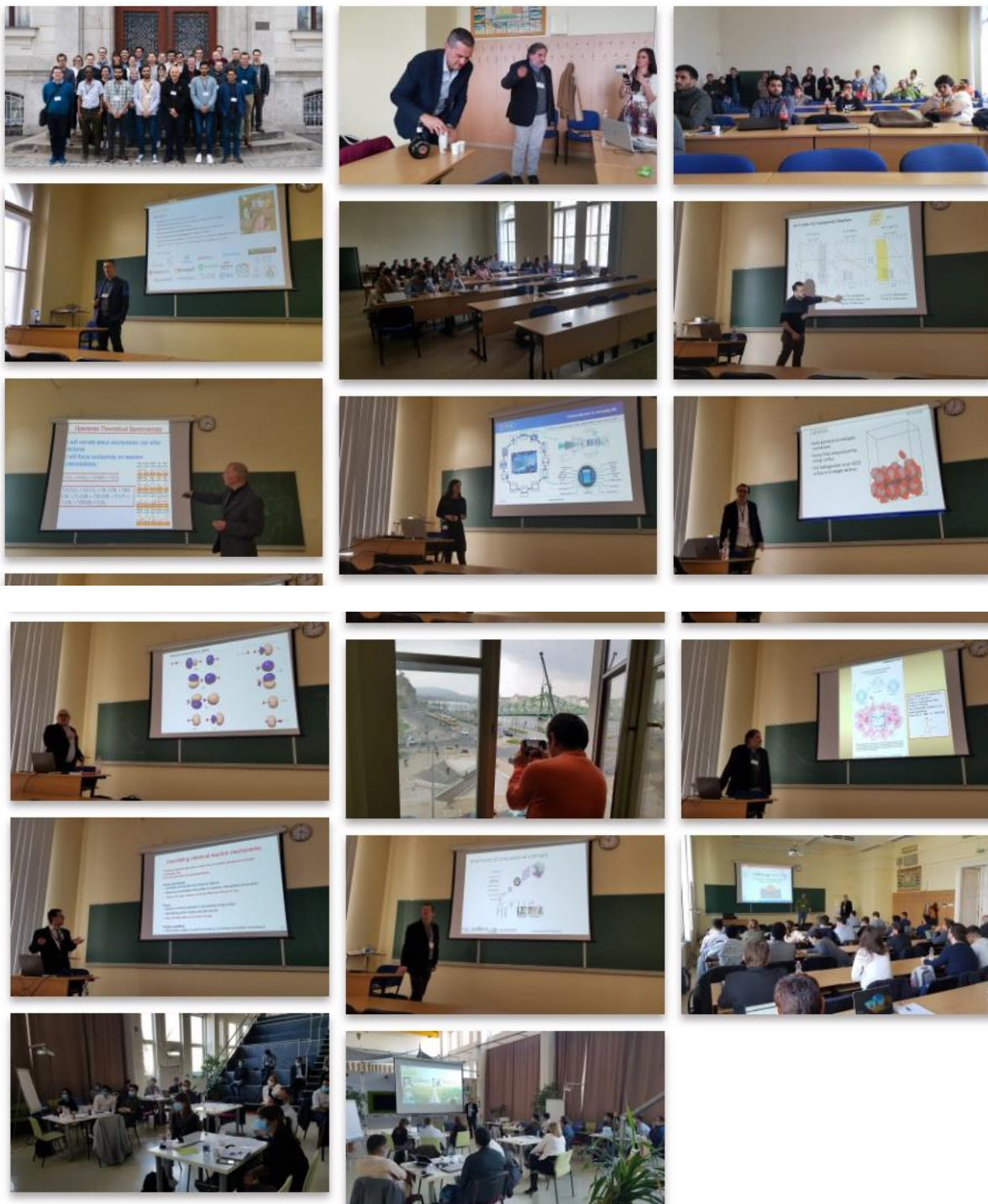
April 21 (Day 3)	Furukawa Electric Institute of Technology Ltd – FETI	Google Map	
09:00 – 09:15	FETI introduction		
09:15 – 09:45	Industrial research and development	Antal Kováts CTO of FETI	
10:00 – 10:45	Practical session: Learn from practice		
	Coffee / Tea Break		
11:15 – 13:00	Practical session: Learn from practice		
	Lunch		
14:00 – 15:45	CO ₂ Capture and Utilization (CCU) Matters: Positioning in the Sustainable Transition Landscape	Metin Bulut VITO, BE	
	Coffee / Tea Break		
16:15 – 18:00	Introduction to intellectual property	Edward Charbonneau OFS Fitel LLC, USA	
	End of First Catchy School		
19:00- 22:00	Dinner Vén Hajó restaurant boat on the Danube	Google Map	

Photo gallery - training



Social Dinner

