# *Scientific Program*

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| **08.15 – 09.00** | **Registration and Breakfast** | |
| **09.00 – 09.20** | **Opening by Professor Jean-François GOHY, Head of the IMCN**<br><br>**ACIM presentation by Pierre-Paul DE BREUCK** | |
| ***Session 1*** | ***Chairman : Professor Michael SINGLETON*** | |
| **09.20 – 09.35** | **Carole BODY**<br>*Control of regioselectivity in the dimerisation of transcinnamic acid and its derivatives using crystal engineering*<br>Supervisor : T. Leyssens | OC1 |
| **09.35 – 09.50** | **Pierre-Paul DE BREUCK**<br>*Uncertainty in data-driven materials science: a case study on MODNet*<br>Supervisor : G.-M. Rignanese | OC2 |
| **09.50 – 10.05** | **Robin GLORIEUX**<br>*Cavity ringdown spectroscopy to probe water-X van der Waals complexes (X = $N_2$, $CO_2$, Ar)*<br>Supervisor : C. Lauzin | OC3 |
| **10.05 – 10.20** | **Quentin PAPELOER**<br>*Effects of PEG on PLLA isothermal crystallization and morphology*<br>Supervisors : S Demoustier & A. Jonas | OC4 |
| **10.20 – 10.35** | **Yonghua TAN**<br>*Discrete palladium complexes-triggered deprotection chemistry in living cells*<br>Supervisors : O. Riant & R. Frédérick | OC5 |
| **10.35 - 10.50** | **Margot VAN DER VERREN**<br>*Innovative Au-Sn-$SiO_2$ bifunctional material for the upgrading of glycerol to methyl lactate*<br>Supervisor : D. Debecker | OC6 |
| **10.50 – 11.20** | ***Poster Session and Coffee Break*** | |

| ***Session 2*** | ***Chairwoman : Professor Sophie HERMANS*** | |
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| **11.20 – 11.35** | **Yousra BAHJOU**<br>*Synthesis of new coordination complexes built by a new family of tetrazole and triazole ligands, Mossbauer and Squid studies of the Iron(II) complex*<br>Supervisor : Y. Garcia | OC7 |
| **11.35 – 11.50** | **Hewei XU**<br>*Alcohol-based electrolytes: an alternative between aqueous and nonaqueous for increased voltage and high-rate lithium-ion batteries*<br>Supervisor : A. Vlad | OC8 |
| **11.50 – 12.05** | **Romain CLAES**<br>*Phonon-limited carrier mobility in semiconductors from first principles*<br>Supervisors : G.-M. Rignanese & G. Hautier | OC9 |
| **12.05 – 12.20** | **Denis DOCHAIN**<br>*Innovative sol-gel routes to bifunctional catalysts for the upgrading of bioethanol to butadiene*<br>Supervisor : D. Debecker | OC10 |
| **12.20 – 12.35** | **Mengyuan DU**<br>*Exploring the chemical space of Fe-$PO_4$-F materials for high performance energy storage*<br>Supervisor : A. Vlad | OC11 |
| **12.35 – 12.50** | **Ashish RAJ**<br>*Polyhydroxy urethanes and carbonates bearing bio-based solid electrolyte for solid-state lithium batteries*<br>Supervisor : J.-F. Gohy | OC12 |

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| **12.50 – 14.25** | ***Lunch and Poster Session*** |
| | ***Discussion with industrial partners (for selected candidates only)*** |

***Session 3*** ***Chairman : Doctor Flavio ABREU ARAUJO***

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| **14.25 – 14.40** | **Nathalie BODY**<br>*Dimethylphenanthroline, a suitable platform for the anchoring of copper photocatalysts*<br>Supervisors : S. Hermans & O. Riant | OC13 |
| **14.40 – 14.55** | **Zehan CHEN**<br>*Hollow porous silicon nanospheres with 3D SiC@C coating as high-performance anodes*<br>Supervisor : J.-F. Gohy | OC14 |
| **14.55 – 15.10** | **Miriam Estefanía CISNEROS GONZÁLEZ**<br>*Modeling the VIS-NIR spectra of Jupiter's Atmosphere with ASIMUT-ALVL*<br>Supervisor : C. Lauzin | OC15 |
| **15.10 – 15.25** | **Maëlle BOTTIN**<br>*Aromatic oligoamides with tunable cavity as receptors for selective anion recognition*<br>Supervisor : M. Singleton | OC16 |
| **15.25 – 15.40** | **Xiaolong GUO**<br>*High voltage organic framework and electrically conducting coordination polymers for high performance alkali-ion batteries*<br>Supervisors : Y. Garcia & A. Vlad | OC17 |
| **15.40 – 15.55** | **Yingrui ZHAO**<br>*$CO_2$ methanation with high loading Ni/$SiO_2$ catalysts prepared by sol-gel method*<br>Supervisor : D. Debecker | OC18 |

**15.55 – 16.25** ***Poster Session and Coffee Break***

***Session 4*** ***Chairman : Professor Xavier GONZE***

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| **16.25 – 16.40** | **Michela MARCHESE**<br>*Reactions of unsaturated acceptors: methodology and applications to functionalization via radical pathways*<br>Supervisor : O. Riant | OC19 |
| **16.40 – 16.55** | **Yuqing HE**<br>*Machine learning on topological electronic materials*<br>Supervisor : G.-M. Rignanese | OC20 |
| **16.55 – 17.10** | **Weiyang LI**<br>*Supramolecular* $Fe^{II}{}_4L_4$ *cage for fast ammonia sensing*<br>Supervisor : Y. Garcia | OC21 |
| **17.10 – 17.25** | **Carla BARAKAT**<br>*Synthesis and characterization of new types of solid polymer electrolytes based on vitrimer-like behavior*<br>Supervisor : J.-F. Gohy | OC22 |
| **17.25 – 17.40** | **Diego MONTESDEOCA ESPIN**<br>*Catalytic conversion of lignocellulose in a "lignin first" biorefinery approach*<br>Supervisor : D. Debecker | OC23 |

**17.40** ***Closing Remarks by Professor Arnaud DELCORTE***

***IMCN Thesis Award by Professor Xavier GONZE***

***Reception***

***Barbecue organized by the ACIM (place Ste-Barbe)***