Annual NISM meeting 2023

Terra Nova, Citadel of Namur
December 18th 2023

Welcome, Prof. Vincent Liégeois: 9:00–9:10

Session 1, chair: Carmela Aprile, Anthony Morena

David Cannella ***(invited Talk)***	"The push-forward role of Biofuels in the modern Biorefinery and in Bio Sustainable society"	9:10–9:50
Julien Bouchat	"Coherent scattering in quasi-ordered structures gives rise to the blue colour of the bluespotted ribbontail ray"	9:50–10:05
Chloé Célis	"Design of bifunctional silica-based nanotubes for the catalytic conversion of carbon dioxide into cyclic carbonates"	10:05–10:20

Flash poster session (3 minutes each)**:** 10:20–10:35

Dorothée Brandt	"Coarse-graining PBTTT, a semi-conducting polymer"
Maxime Mathieu	"Towards Shape-Tunable Hierarchical TiO_2 Single Crystals as Catalyst for CO_2 Valorization"
Komlanvi Sèvi Kaka	"Third-order nonlinear optical properties of organic p-conjugated molecules: quantum chemistry studies and comparison with experiment"
Vittorio Marsala	"Towards the understanding of the formation mechanism of hollow silica nanotubes and nanospheres: an NMR approach"
Nicolas Niessen	"Development and Lewis Acidity of Pyramidal Triarylborane and Borenium Ions"

Coffee break and poster session: 10:35–11:00

Session 2, chair: Emile Haye

Mathias Fraiponts	"Rational Design and Synthesis of Pyrrolopyrrole Aza-BODIPY Photosensitizers for Image-Guided Photodynamic Therapy"	11:00–11:15
Alireza Bagherpour	"Vein pattern vs. columnar fracture shape in Cu-Zr thin film metallic glasses: Driving force and mechanism"	11:15–11:30
Xikun Zhang	"Dual ions co-intercalation induced spontaneous and reversible phase replacement chemistry enables superior Zn^{2+} storage"	11:30–11:45
Danillo Pires Valverde	"Computational Insights into the Photophysics of Inverted Singlet-Triplet Gap Materials"	11:45–12:00

Intervention de Murielle Guillaume,
responsable cellule emploi du SRH de l'UNamur: 12H00–12H30

Lunch and poster session: 12:30–13:35

Session 3, chair: Yoann Olivier, Gaetano Ricci

Claire Tonnelé ***(invited Talk)***	"Chasing neutrino's nature: Ba^{2+} luminescent sensing from a computational perspective"	13:35–14:15
Nicolas Roy	"Utilizing highly data-efficient computational intelligence for the engineering of photonic devices: a case study on vortex phase mask coronagraphs"	14:15–15:30
Kajetan Bijouard	"B-YOND: Reprogramming the reactivity of main-group elements"	15:30–14:45
Loris Chavée	"Growth mechanisms and properties of magnetron sputtered TiO_2 thin films on complex 3D foam substrates"	14:45–15:00

Coffee break and poster session: 15:00–15:25

Session 4, chair: Francesca Cecchet

Adrien Debacq	"Crystal Clear Dirac Cone Prediction in Photonic Band Structures"	15:25–15:40
Mohamed Achehboune	"Atomistic insights into nucleation and growth of hexagonal Boron Nitride on Germanium"	15:40–15:55

Conclusions, Prof. Francesca Cecchet: 15:55–16:00
Drink: 16:00–17:00

Poster sessions

Mohamed Chellegui	"Exploring Reaction Mechanism of Diels-Alder Cycloadditions between Furan-Based Dienes and Ethylene Derivatives. A Study from the Perspective of Bond Evolution Theory"
Jun Chen	"Inverse opal material photocatalyst for enhanced light absorption facilitates photocatalytic conversion of renewable and low value biomass into value-added chemicals"
Lou D'haese	"Surrounding effects on Raman optical activity signatures"
Alban de Gary	"Maximizing light outcoupling in OLEDs: insights from molecular simulations"
Oliver Garot, Anthony Morena	"Understanding the acidity properties of different silica-based materials via ^{31}P ssNMR using TMP as probe molecule"
Laurelenn Hennaux	"Structural and functional characterization of a copper efflux membrane protein: PcoB from Caulobacter crescentus"
Valentin Job	"Investigation of the Antimicrobial Properties of Thin Films Produced by Low Pressure Magnetron"
Jing Li	"Hierarchical Heterostructured Cathode for a Visible-Light-Involved in Lithium–Oxygen Battery"
Zhonghao Miao	"Tailoring short-chain sulfur molecules to drive redox dynamics for sulfur-based aqueous battery"
Thanh Trung Pham	"Investigation of 1H-MoTe2 doped with nitrogen"
Gaetano Ricci	"Exploring the electronic structure of extended triangulenes: opening new doors for a fast Reverse Intersystem Crossing"
Martina Saitta	"Conversion of glycerol into solketal catalyzed by hybrid porous zirconium(IV) phosphonate networks"
Tanguy Scaillet	"Towards the Development of Covalent Inhibitors for Brucella Militensis SerB through Crystallography and Kinetics"
Laura Valentino, Chloé Célis	"Phosphonium Salt/Al-Porphyrin Copolymer as Bifunctional Heterogeneous Catalyst for CO_2 Conversion to Cyclic Carbonates"
Guanying Wang	"Synthesis of Hierarchical Single-Crystal ZSM-5 and SAPO-34 Zeolite"
Yuanguo Wu	"Sharing Electronic and Ion Transfer Channels by In-Situ Integration of Gel Polymer Electrolyte for Solid-State Lithium-Oxygen Battery"
Hao Xu	"Impact of Mo/W distribution on the properties of Keggin catalysts"
Liuxi Yang	"Non-covalently synthesis of porous organic salts"
Runtian Zheng	"Integrated insights into NH_4^+ storage mechanism and electrochemical kinetics of ultrastable Prussian blue analogues for Ammonium-Ion Battery"