

9^e journée scientifique de l'école doctorale thématique METAMORPHOSE

Vendredi 26 mai 2023

Université Libre de Bruxelles
Salle Solvay (Campus Plaine)

8h45 WELCOME

9h25 Introduction

Chair: [Pascal KOCKAERT \(Université Libre de Bruxelles\)](#)

9h30 **Bart KUYKEN** (Ghent University, Photonics Research Group) (**invited speaker**): *Chip scale electrically powered optical frequency combs.*

10h15 **Helena CARVAJAL GALLEGÓ** (Université de Mons): *Atomic structure and opacity calculations in moderately ionized lanthanides for modeling kilonova spectra.*

10h35 **Maarten KONINGS** (Katholieke Universiteit Leuven): *Representations of the three lowest $^2A'$ adiabatic electronic potential energy surfaces for the ArH_2^+ reactive system with machine learning.*

10h55 COFFEE BREAK and POSTERS

Chair: [Pascal QUINET \(Université de Mons\)](#)

11h30 **Nicolas CALLEBAUT** (Université Libre de Bruxelles): *Quantum mechanical study of size and sequence effects on the ionization potential of stacked DNA bases.*

11h50 **Joffrey FREREUX** (Université Catholique de Louvain): *Action spectroscopic study of $(\text{H}_2\text{O}-\text{X})^+$ complexes in the overtone range.*

12h10 **Antoine AERTS** (Université Libre de Bruxelles): *The nature of molecular vibrations: theoretical investigation and use in laser quantum control.*

12h30 LUNCH (sandwich buffet) and POSTERS

Chair: Nathalie VAECK (Université Libre de Bruxelles)

13h30 **Jean Christophe TREMBLAY** (CNRS – Université de Lorraine, Metz, France) (**invited speaker**): *Theoretical investigation of metastable polyfluoride anions via matrix isolation spectroscopy.*

14h15 **Simon COLLIGNON** (Université Catholique de Louvain): *Instrumental development of a CP-FTMW spectrometer at UCLouvain for spectroscopic studies in the 6–18 GHz frequency range.*

14h35 **Thibault BERTIN** (Université Libre de Bruxelles): *CO₂ collision-induced line parameters for the ν₃ band of CH₄ measured using a hard-collision speed-dependent line shape and the relaxation matrix formalism.*

14h55 COFFEE BREAK and POSTERS

Chair: Clément LAUZIN (Université Catholique de Louvain)

15h30 **Lucile RUTKOWSKI** (Université de Rennes, France) (**invited speaker**): *Frequency combs in high resolution molecular spectroscopy: From metrology to astrochemistry applications.*

16h15 **Miriam CISNEROS** (Université Catholique de Louvain, Institut d'Aéronomie Spatiale de Belgique): *Modelling aerosols in Jupiter's atmosphere with ASIMUT-ALVL.*

16h35 **Bonah LUIS** (I. Physikalisches Institut, Universität zu Köln, Germany): *Leveraging double-resonance spectroscopy to understand trans-glyceraldehyde and seventeen of its vibrationally excited states.*

16h55 FINAL REMARKS

17h00 END OF MEETING

POSTERS

B. Bertrand;¹ *The BOOSTED network: Belgium Optical network for Optical frequency Standards and TimE Dissemination.*

J. Clément,² N. Dricot,² B. Vispoel,² O. Browet,² M. Mangold,³ J. Hayden,³ P. Allmendinger,³ A. Hugi,³ M. Lepère;² *CO₂- and N₂-collisional broadening coefficients of lines in the ν₄ band of methane by mid-infrared dual-comb spectroscopy.*

S. Ghose,⁴ M.A. Cardosa,⁴ F. Remacle;⁴ *Effect of tethering on the mechanical response of weak bond complexes.*

K. Leroux,⁵ A. Rizopoulos,⁵ J. Vander Auwera;⁵ *IR absorption cross sections of organic molecules in support to the exploration of planetary atmospheres.*

L. Maison,⁶ M. Godefroid,⁵ P. Palmeri,⁶ P. Quinet,^{6,4} *Multiconfiguration Dirac-Hartree-Fock calculations of the A hyperfine constant for the ground state of 137-Ba II.*

E. Marin Bujedo;⁷ *Theoretical study of the l-dependence of the auto-ionization rates of core-excited Rydberg states.*

R. Marion,⁷ M. Terao-Dunseath,⁸ K.M. Dunseath,⁸ X. Urbain;⁷ *Absolute cross sections and asymmetry parameters for photodetachment of excited C⁻ (2D).*

P. Misra,⁹ B. Heyne,⁹ G. Grutzeck,⁹ M. Fatima,⁹ S. Schlemmer;⁹ *New horizons for taking rotational spectra of astrophysically relevant molecules.*

L. Yang,² B.-L. Su;² *Non-covalently synthesis of porous organic salts.*

(1) Observatoire Royal de Belgique ; **(2)** Université de Namur ; **(3)** IRsweep (Switzerland) ; **(4)** Université de Liège ; **(5)** Université Libre de Bruxelles ; **(6)** Université de Mons ; **(7)** Université Catholique de Louvain ; **(8)** Université de Rennes ; **(9)** Universität zu Köln.