

WINTER MODELING

A SPECIAL EDITION:

Vincenzo Barone and his 70th birthday

10-11 November 2022



SSM
Scuola Superiore Meridionale

An international workshop in honor of Prof. Vincenzo Barone

WELCOME AND INTRODUCTION

PROF. MATTEO LORITO – RECTOR, UNIVERSITÀ DEGLI STUDI DI NAPOLI FEDERICO II

PROF. LUIGI AMBROSIO – DIRECTOR, SCUOLA NORMALE SUPERIORE

PROF. ARTURO DE VIVO – GOVERNANCE, SCUOLA SUPERIORE MERIDIONALE

INVITED SPEAKERS

Carlo Adamo (Laudatio) École Nationale Supérieure de Chimie de Paris (France)

José Luis Alonso Universidad de Valladolid (Spain)

Malgorzata Biczysko University of Shanghai (China)

Julien Bloino Scuola Normale Superiore (Italy)

Alessandro Fortunelli Consiglio Nazionale delle Ricerche (Italy)

Laura Gagliardi University of Chicago (USA)

Claudio Greco Università degli Studi Milano-Bicocca (Italy)

Marco Pagliai Università degli Studi di Firenze (Italy)

Michele Pavone Università degli Studi di Napoli Federico II (Italy)

Nino Russo Università della Calabria (Italy)

Mauro Stener Università degli Studi di Trieste (Italy)

JUNIOR SCIENTISTS

Silvia Alessandrini Alma Mater Studiorum Università di Bologna (Italy)

Federico Lazzari Scuola Normale Superiore, Pisa (Italy)

Fulvio Perrella Scuola Superiore Meridionale, Napoli (Italy)

Scientific & Organizing Committee

Nadia Rega

(chair, Università degli Studi di Napoli Federico II)

Cristina Pizzarini

(co-chair, Alma Mater Studiorum Università di Bologna)

Marco Mendolicchio

(Scuola Superiore Meridionale, Napoli)

Scientific Secretary - Contact

Marinella Rotondo

(Associazione Le Minerve)

Conference Center of the University of Naples Federico II (Lecture Hall A)

Via Partenope 36, Naples

10 NOVEMBER 2022

14:00 REGISTRATION

14:45 OPENING: WELCOME & INTRODUCTION

PROF. MATTEO LORITO *Rector, Università degli Studi di Napoli Federico II*

PROF. LUIGI AMBROSIO *Director, Scuola Normale Superiore*

PROF. ARTURO DE VIVO *Governance, Scuola Superiore Meridionale*

15:20 WELCOME «BRINDISI»

SESSION 1 (CHAIR: N. REGA)

16:00 CARLO ADAMO *Laudatio*

16:45 LAURA GAGLIARDI

Engineering Metal Organic Framework Functionalities Using Theory, Computations and High-Throughput Data

JUNIOR SESSION (CHAIR: S. COLUCCIA)

17:30 POST-DOCS

SILVIA ALESSANDRINI

Intersystem Crossing in the Entrance Channel of the Reaction between $O(^3P)$ and Pyridine

FEDERICO LAZZARI

The Virtual Laboratory

FULVIO PERRELLA

Ultrafast Photo-induced Processes in Dye Sensitizers: Insight from Theory

18:30 PHD STUDENTS (ASTROCHEMISTRY & MOSES)

L. CRISCI *On the Automation of VRC-TST Simulations: Strategies to Determine Wave Function Guesses, Exploration of Black-box Methodologies, and Application to Test Systems*

G. IUZZOLINO *Unraveling the Photophysics of a Prototype System for DNA-Protein Photocrosslinking*

A. MELLI *Spectroscopic Characterization of 3-Aminoisoxazole: a Prebiotic Precursor of Ribonucleotides*

E. ROMANO *Stereo-Electronic Effects in Olefin Polymerization Catalysis analyzed by Energy Decomposition of Density Functional Computations*

20:30 SOCIAL DINNER

11 NOVEMBER 2022

SESSION 2 (CHAIR: S. ABBATE)

9:00 **JOSÉ LUIS ALONSO**

Watching Biomolecules: A Joint Venture of Quantum Chemistry and Rotational Spectroscopy

9:45 **MALGORZATA BICZYSKO**

Computational Spectroscopy: from Mid Infrared (MIR) to Vacuum Ultraviolet (VUV)

10:30 **MAURO STENER**

New TDDFT Algorithms, Protocols and Analysis Tools for the Study of Optical Properties of Large Metal Nanoclusters

11:15 **COFFEE BREAK**

SESSION 3 (CHAIR: G. TALARICO)

11:45 **MARCO PAGLIAI**

Structure and Dynamics of Hydrogen Bonded Systems from Molecular Dynamics Simulations

12:30 **JULIEN BLOINO**

Good Vibrations - A Journey in Search of Efficient Models to Describe Accurately Nuclear Contributions

13:15 **FREE LUNCH**

SESSION 4 (CHAIR: M. MENDOLICCHIO)

15:00 **CLAUDIO GRECO**

Theoretical Studies of Chemical Systems with Environmental Relevance: Gas-processing Enzymes, Biomimetic Catalysts and Green Nanoreactors

15:45 **MICHELE PAVONE**

When Molecules Meet Materials: A Quantum Chemical Perspective on Heterogeneous Functional Interfaces

16:30 **COFFEE BREAK**

SESSION 5 (CHAIR: C. PUZZARINI)

17:00 **ALESSANDRO FORTUNELLI**

Simulation Studies of Dynamic Processes in Catalysis and Materials Science

17:45 **NINO RUSSO**

Computational Enzymology on the Road

18:30 **CLOSING REMARKS**



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