

Program of the 3rd General Meeting of the COSY Cost Action

Wednesday 9/7		Thursday 10/7		Friday 11/7	
8:30-9:20	Registration + Opening	8:30-9:00	Registration	9:00-9:30	Registration
9:20-10:00	Mattia Melosso	9:00-9:40	Alessandro Fortunelli		
10:00-10:25	Vladimir Sreckovic	9:40-10:05	A. Sezai Sarac	9:30-10:10	Berta Fernandez Rodriguez
10:25-10:50	Malgorzata Biczysko	10:05-10:30	Michele Reticcioli	10:10-10:35	Piotr Żuchowski
10:50-11:15	Alberto García-Vela	10:30-10:55	Aggelos Avramopoulos	10:35-11:00	Vincenzo Barone
11:15-11:45	Coffee break	10:55-11:25	Coffee break	11:00-11:30	Coffee break
11:45-12:10	Justyna Krupa	11:25-11:50	Stefan Vajda	11:30-11:55	Markus Meuwly
12:10-12:30	Alessandra Savarese (YR-PhD)	11:50-12:30	Maria Pilar de Lara Castells	10:55-12:15	Dennis Dinu (YR)
12:30-12:50	Petra Čechová (YR)	12:30-12:45	Javier Hernández Rodríguez (YR-PhD)	12:15-12:45	Denis Comte (YR)
12:50-13:05	Markéta Paloncýová (YR)	12:45-14:30	LUNCH	12:35-14:30	LUNCH
13:05-14:50	LUNCH				
14:50-15:30	Majdi Hochlaf	14:30-16:30	Management Committee Meeting	14:30-14:50	Luigi Crisci (YR)
15:30-15:55	Jorge Marques			14:50-15:10	Silvia Alessandrini (YR)
15:55-16:20	Kęstutis Aidas			15:10-15:35	Sergiy Perepelytsya
16:20-16:35	Einaras Sipavičius (YR-PhD)			15:35-16:00	Ljiljana Suručić
16:35-17:05	Coffee break	16:30-17:00	Coffee break	16:00-16:10	Closing remarks
17:05-17:30	Sandra Gomez Rodriguez	17:00-18:20	Management Committee Meeting	16:10-18:00	Aperitif & Farewell
17:30-17:55	Miroslav Medved'				

Wednesday 9/7

9:20-10:00	Mattia Melosso	<i>Rotational spectroscopy of potentially detectable interstellar molecules. (E)-1-propenol as an example.</i>
10:00-10:25	Vladimir Sreckovic	<i>Exploring Confined Molecular Systems and Their Role in Astrochemical Processes</i>
10:25-10:50	Malgorzata Biczysko	<i>Reliable modeling of anharmonic spectra from VPT2 and hybrid QM models</i>
10:50-11:15	Alberto García-Vela	<i>Quantum Control of the Dynamical Behavior of Resonance States in Small Organic Molecules with Intense Fields</i>
11:15-11:45	Coffee break	
11:45-12:10	Justyna Krupa	<i>Studies of Weak Complexes with Atmospheric and Astrochemical Relevance in Cryogenic Confinement: Where Experiment Meets Theory</i>
12:10-12:30	Alessandra Savarese (YR-PhD)	<i>Identification of the Best Candidates for Radioastronomical Detection within the C₃H₆O₂ Isomer Family</i>
12:30-12:50	Petra Čechová (YR)	<i>Cholesterol effect on the phase of lipid crowded environment</i>
12:50-13:05	Markéta Paloncýová (YR)	<i>Simulation Insight into Confined Lipid-based Systems</i>
13:05-14:50	LUNCH	
14:50-15:30	Majdi Hochlaf	<i>Molecular confinement induced effects: structures, spectroscopies, reactivity and applications</i>
15:30-15:55	Jorge Marques	<i>From the computational study of protein-ligand confined systems to the design of pesticides-adsorbing materials</i>
15:55-16:20	Kęstutis Aidas	<i>Towards Accurate Modelling of ¹H NMR Spectra of Ionic Liquid</i>
16:20-16:35	Einaras Sipavičius (YR-PhD)	<i>Intermolecular Organization In Aqueous Mixtures Of Choline Lysinate Studied By NMR And Molecular Dynamics/Quantum Mechanics</i>
16:35-17:05	Coffee break	
17:05-17:30	Sandra Gomez Rodriguez	<i>Methods to study deactivation of excited states in condensed systems</i>
17:30-17:55	Miroslav Medved'	<i>Iminothioindoxyls: A New Class of Molecular Photoswitches</i>

Thursday 10/7		
9:00-9:40	Alessandro Fortunelli	<i>High-Throughput and Conformal Funnels in NanoCatalytic Processes</i>
9:40-10:05	A. Sezai Sarac	<i>Polyacrylonitrile Composite Nanofibers with Confined Magnetic Ferrite Nanoparticles</i>
10:05-10:30	Michele Reticcioli	<i>Machine Learning for Polaronic Materials: TiO₂(110) at the nanoscale</i>
10:30-10:55	Aggelos Avramopoulos	<i>Hyperpolarization Effects in Molecular Materials</i>
10:55-11:25	Coffee break	
11:25-11:50	Stefan Vajda	<i>Addressing Size, Composition and Support Effects in Nanocatalysis: Subnanometer Mono- and Bimetallic Clusters in CO Oxidation</i>
11:50-12:30	Maria Pilar de Lara Castells	<i>Unsupported and surface-supported subnanometric metal clusters as fluxional Jahn-Teller molecules</i>
12:30-12:45	Javier Hernández Rodríguez (YR-PhD)	<i>Non-Adiabatic Dynamics of Excited States in Tetraphenylpyrazine: From Monomer to Dimer</i>
12:45-14:30	LUNCH	
14:30-16:30	Management Committee Meeting	
14:30-16:30	Coffee break	
17:00-18:20	Management Committee Meeting	

Friday 11/7

9:00-9:30	Registration	
9:30-10:10	Berta Fernandez Rodriguez	<i>Pursuing Accuracy in the Evaluation of Intermolecular Potentials</i>
10:10-10:35	Piotr Żuchowski	<i>Response theory and molecular interactions</i>
10:35-11:00	Vincenzo Barone	<i>Next-Gen Computational Spectroscopy with VMS2.0: Accurate, AI-Enhanced, Scalable, and User-Friendly</i>
11:00-11:30	Coffee break	
11:30-11:55	Markus Meuwly	<i>Machine Learning Based Potential Energy Surfaces for Chemical Reactions</i>
10:55-12:15	Dennis Dinu (YR)	<i>Seven Years in the Matrix: A Personal Journey Through Cryogenic Spectroscopy and Vibrational Theory</i>
12:15-12:45	Denis Comte (YR)	<i>Protonated Dimers as Gateways to Interstellar Chemical Evolution</i>
12:35-14:30	LUNCH	
14:30-14:50	Luigi Crisci (YR)	<i>DDCI-Augmented PCS Protocol: Unlocking Size-Consistent, Near-Full-CI Accuracy in Bond Dissociation Reactions</i>
14:50-15:10	Silvia Alessandrini (YR)	<i>Formation of glycolamide (NH₂C(=O)CH₂OH) on interstellar ice grains: Insights from atomistic simulations</i>
15:10-15:35	Sergiy Perepelytsya	<i>Counterion-induced DNA confinement: Modeling and simulation insights for biological and nanotechnological applications</i>
15:35-16:00	Ljiljana Suručić	<i>Bridging the Gap: Challenges and Opportunities for Bosnian-Herzegovinian Participation in COST Actions</i>
16:00-16:10	Closing remarks	
16:10-18:00	Aperitif & Farewell	

Lunch Menu on Wednesday 9/7 (Vegetarian Option indicated with 🌿)

Finger Food:

1. Piccoli spiedini di mozzarelline di bufala e pomodorini ciliegini 🌿
Vegetarian skewers with mozzarella and cherry tomatoes
2. Bocconcini soffici alle olive farciti con crudo dolce di Parma
Soft mini-bread with Parma Ham and olives
3. Rombetti di frittata ai sapori di campo 🌿
Small slices of omelette with spinach
4. Piccoli tramezzini assortiti
Small sandwiches
5. Torta salata vegetariana con ricotta e spinaci 🌿
Quiche with ricotta and spinach
6. Crocchettine di patata 🌿
Potato croquettes
7. Crostini dorati ai sapori di bosco 🌿
Tosted bread with veggies and mushrooms

Main Course:

1. Mezze maniche con pomodorini ciliegini, basilico e bruciatini di pancetta
Pasta with cherry tomato, basil and bacon
2. Rosette verdi con fontina, melanzane e basilico 🌿
Oven cooked egg and spinach pasta with cheese, aubergines and basil

Desserts:

1. Frutta fresca di stagione 🌿
Seasonal fruit
2. Ciotolini di mousse al pistacchio di Bronte 🌿
Small bowls of pistachio mousse

Lunch Menu on Thursday 10/7 (Vegetarian Option indicated with 🌿)

Finger Food:

1. Piccoli spiedini di mozzarelline di bufala e pomodorini ciliegini 🌿
Vegetarian skewers with mozzarella and cherry tomatoes
2. Piccoli sandwich a bocca di lupo farciti con salumi e salsine
Small sandwiches with cold cuts and sauces
3. Bicchierino con tarallini pugliesi, stracchino, basilico e pomodorini confit 🌿
Bowls with "tarallini", soft cheese, basil and confit tomatoes
4. Mini calzoncini vegetariani con ricotta e spinaci 🌿
Toasted bread with ricotta and spinach
5. Focaccine farcite con melanzane grigliate e mozzarella 🌿
Focaccia bread with aubergine and mozzarella
6. Bruschettine dorate con speck e zucchine marinate
Toasted bread with speck and courgette
7. Piccolo stecchino alla bolognese pastellato
Fried Bologna-meat skewers

Main Course:

1. Pennette con fiammiferi di speck, asparagi e zafferano
Pasta with speck, asparagus and saffron
2. Crespelle delicate ai sapori di bosco su fonduta di Parmigiano Reggiano 🌿
Oven-cooked crepes with mushrooms and parmesan

Desserts:

1. Frutta fresca di stagione
Seasonal fruit
2. Ciotolini di tiramisù
Small bowls of tiramisù

Lunch Menu on Friday 11/7 (Vegetarian Option indicated with 🌿)

Finger Food:

1. Piccoli spiedini di mozzarelline di bufala e pomodorini ciliegini 🌿
Vegetarian skewers with mozzarella and cherry tomatoes
2. Piccoli sandwich a bocca di lupo farciti con salumi e salsine
Small sandwiches with cold cuts and sauces
3. Mini calzoncini con prosciutto cotto e fontina
Small stuffed "calzone" with ham and cheese
4. Rombetti di frittata ai sapori di campo 🌿
Small slices of omelette with spinach
5. Quiche Lorraine con mozzarella, funghi e prosciutto cotto
Quiche with mozzarella, mushrooms and ham
6. Bruschettine dorate con speck e zucchine marinate
Toasted bread with speck and courgette
7. Crocchettine di patata 🌿
Potato croquettes

Main Course

1. Cous cous con ratatouille di verdure ripassate al forno 🌿
Cous Cous with roasted veggies
2. Nidi di rondine alla Romagnola con prosciutto cotto e fontina
Roasted egg-pasta with ham and cheese

Desserts:

1. Frutta fresca di stagione 🌿
Seasonal fruit
2. Sacher torte monoporzione 🌿
Sacher torte