

XLIX Congress of the Physical Chemistry Division of the Società Chimica Italiana

Physical Chemistry: a fresh glimpse into
the microscopic world



Torino 4-7 September 2023



Local Organizing Committee

P. Ugliengo – Chair

A. Damin

F. Bonino

S. Casassa

A. M. Ferrari

L. Maschio

G. Ricchiardi

V. Crocellà

S. Bordiga

B. Civalleri

E. Groppo

L. Mino

D. Scarano

M. Corno

G. Berlier

E. Borfecchia

A. Erba

G. Magnacca

S. Morandi

M. Signorile

Scientific Committee

M. Meneghetti - Chair

S. Brutti

M. Ferretti

G. Marletta

L. Petraccone

A. Polo

F. Ridi

M. L. Saladino

P. Ugliengo

F. Zerbetto

Collane@unito.it

Università degli Studi di Torino

ISBN: 9788875902704

This work is licensed under [CC BY-SA 4.0](https://creativecommons.org/licenses/by-sa/4.0/) 

Publication date: 25-08-2023



WELCOME IN TURIN

Welcome to the **49th National Congress of Physical Chemistry** (XLIX CNCF, Turin 2023), promoted by the **Physical Chemistry Division of the Società Chimica Italiana**.

The Conference, organized by the Physical Chemists of the University of Turin, is be hosted by the Department of Molecular Biotechnology and Health Sciences.

The aim of the conference is to show how the physical-chemical approach, based on a multi-scale view of matter, offers fundamental contributions, through experimental, theoretical and computer modeling methodologies, in fields ranging from astrochemistry, biochemistry, catalysis, soft-matter to materials science (to name but a few).

The scientific program is divided into six thematic sessions, introduced by plenary lectures by researchers who will demonstrate the synergy between experimental and theoretical methods in understanding the fundamental mechanisms of chemistry

Activities open to the public, dedicated to topics of general interest, will be offered during the conference.

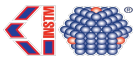
Social events will make your stay more enjoyable with additional opportunities for an informal exchange of ideas.



PATRONAGE & SPONSORS

Sponsors

Patronage





GENERAL INFORMATION

Venue

University of Turin UniTO
Dept. of Molecular Biotechnology and Health Sciences
Via Nizza 52, 10126 Torino

Wifi

Participants can access the wi-fi infrastructure by using the personal Eduroam account. Please check the service has been activated on your devices.

SOCIAL PROGRAMME

Welcome Party

Monday 4 September, 2023 - h 18:30

University of Turin UniTO
Dept. of Molecular Biotechnology and Health Sciences
Via Nizza 52, 10126 Torino

Public Engagement

Tuesday 5 September, 2023 - h 18:00

Clima ed energia: quali scelte per il futuro?

Cavallerizza Reale
Via Giuseppe Verdi 9, 10124 Torino

Social Dinner

Wednesday 6 September, 2023 - h 20:00

Esperia Restaurant
Corso Moncalieri 2, 10131 Torino
(Only with reservation)

Technical Secretariat



EVENTually Meetings & Events
info@eventuallyevents.it
www.eventuallyevents.it
phone + 39 327 3752740

Clima ed energia: quali scelte per il futuro?

Gli effetti della crisi climatica sono già sotto i nostri occhi. Per mitigare quelli futuri e provare a rallentarla, un passaggio fondamentale riguarda il modo in cui produciamo energia. Dobbiamo quanto prima azzerare le emissioni: le fonti rinnovabili sono la principale risposta. Il nucleare continuerà ad avere un ruolo, ma le scelte non potranno che essere diversificate in base alle peculiarità delle diverse regioni del mondo. Che cosa dobbiamo aspettarci? Su quali tecnologie è meglio investire? La ricerca fornirà nuove soluzioni in grado di cambiare gli scenari?

Martedì 5 Settembre 2023

Aula Magna Cavallerizza Reale
Via Giuseppe Verdi, 9 – Torino

Con **Nicola Armaroli**, chimico e Dirigente di Ricerca Consiglio Nazionale delle Ricerche CNR Bologna, **Elisa Palazzi**, climatologa, dipartimento di Fisica dell'Università di Torino e **Daniele Tomatis**, R&D manager di newcleo Futurable Energy, esperti rispettivamente di energie rinnovabili, cambiamento climatico e nucleare di 4^a generazione.

Modera **Alberto Agliotti**, divulgatore scientifico.

www.settimanedellascienza.it

Organizzato da



Nell'ambito di



In collaborazione con





PROGRAMME AT A GLANCE

DARWIN Room

LEONARDO Room

ARISTOTELE Room

Room DARWIN

Time	Monday 04
8:30	Registration
9:30	Welcome
Chair	<i>Civalleri</i>
10:30	Tkatchenko T4
11:15	Alessio (T4)
11:30	Caruso (T4)
11:45	Grobas Illobre (T4)
12:00	Maltoni (T1)
12:15	Silmani (T1)
12:30	Armetta (T1)
13:00	Light lunch
Chair	<i>Polo</i>
14:30	Auditore (T1)
14:45	Baricic (T1)
15:00	Tielens (K-T4)
15:30	Calvino (T1)
15:45	Coffee break & poster
16:30	Flash communication
18:30	Welcome Party

Time	Tuesday 05
Chair	<i>Bordiga</i>
9:00	Dini T3
9:45	Litti (T1)
10:00	Locardi (T1)
10:15	Martini (T1)
10:30	Coffee break & poster
Chair	<i>Ridi</i>
11:30	Melani (T1)
11:45	Miranda Murillo (T1)
12:00	Pavan (K-T1)
12:30	Mudassir (T1)
12:45	Negro (T1)
13:00	Light lunch
Chair	<i>Tielens</i>
14:30	Diebold T1
15:15	Rizzuto (T4)
15:30	Nicoli (T4)
15:45	Invernizzi (T4)
16:00	Pavone (T4)
16:15	Coffee break & poster
18:00	Public engagement

Time	Wednesday 06
Chair	<i>Selli</i>
9:00	Nova T5
9:45	Bocus (T5)
10:00	Bonacchi (T5)
10:15	Campisi (T5)
10:30	Coffee break & poster
Chair	<i>Brutti</i>
11:45	Delle Piane (T5)
12:00	Damin (K-T5)
12:30	Agostini (T3)
12:45	Bartoli (T3)
13:00	Light lunch
Chair	<i>Petraccone</i>
14:30	Elia (T3)
14:45	Grigioni (T3)
15:00	Labarile (T3)
15:15	Lionello (T3)
15:30	Sponsors
16:30	Coffee break & poster
17:00	Assemblea divisione
20:00	Social dinner

Time	Thursday 07
Chair	<i>Pavan</i>
9:00	Mennucci T2
9:45	Alberti (T2)
10:00	Baglioni (T2)
10:15	Campanile (T2)
10:30	Coffee break & poster
Chair	<i>Berlier</i>
11:30	Campione (T2)
11:45	Casale (T2)
12:00	Lambert (K-T2)
12:30	D'Aria (T2)
12:45	Artini (T6)
13:00	Light lunch
Chair	<i>Zerbetto</i>
14:30	Graziano (K-T6)
15:00	Baratta (T6)
15:15	Barbon (T6)
15:30	Coffee break & poster
16:15	Balucani T6
17:00	Casu (T6)
17:15	S. Ferrero (T6)
17:30	Closing remarks

DARWIN

LEONARDO

Room LEONARDO

Time	Monday 04
Chair	<i>Greco</i>
11:30	Zoccante (T4)
12:00	Tabacchi (T4)
12:30	Duce (T1)
12:45	Gallo (T1)
13:00	Light lunch
Chair	<i>Coluccia</i>
14:15	Garroni (T1)
14:30	Peddis (K-T1)
15:00	Grandolfo (T1)
15:15	Lettieri (T1)
15:45	Coffee break & poster
16:30	Flash communication
18:30	Welcome Party

Time	Tuesday 05
Chair	<i>Giovannini</i>
9:45	Scardaci (T1)
10:00	Abdolrahimi (T1)
10:15	Spampinato (T1)
10:30	Coffee break & poster
11:30	Toffoletti (T1)
11:45	Vandenhoute (T1)
12:00	Polo (T3)
12:15	Pierini (T3)
12:30	Narzi (K-T2)
13:00	Light lunch
Chair	<i>Condorelli</i>
15:15	Perrone (T3)
15:30	Romagnoli (T3)
15:45	Sassone (T3)
16:15	Coffee break & poster
18:00	Public engagement

Time	Wednesday 06
Chair	<i>Avanzini</i>
9:45	Papatola (T5)
10:00	Pareras Niell (T5)
10:15	Giannetti (T2)
10:30	Coffee break & poster
Chair	<i>Graziano</i>
12:00	Salvestrini (T5)
12:15	Zeppilli (T5)
12:30	Pamigotto (T5)
12:45	Gianotti (T5)
13:00	Light lunch
14:30	Cioni (T5)
14:45	Dosa (T5)
15:00	Bodo (K-T3)
16:30	Coffee break & poster
20:00	Social dinner

Time	Thursday 07
Chair	<i>Bisio</i>
9:45	R. Ferrero (T2)
10:00	Pioppi (T2)
10:15	Rizzi (T2)
10:30	Coffee break & poster
11:30	Avanzini (K-T6)
12:00	Martinez-Bachs (T6)
12:15	Maris (T6)
12:30	Mannucci (T6)
12:45	Melandri (T6)
13:00	Light lunch
Chair	<i>Maschio</i>
14:30	Miglio (T6)
14:45	Perrero (T6)
15:00	Mino (K-T3)
15:30	Coffee break & poster
17:00	Tavani (T6)
17:15	Vanuzzo (T6)

Room ARISTOTELE

Time Monday 04	
Chair	<i>Mino</i>
11:45	Pedone (T4)
12:00	Giovannini (K-T4)
12:30	Corsaro (T1)
12:45	Ribaldone (T4)
13:00	Light lunch
Chair	<i>Lambert</i>
14:30	D'Agostini (T1)
14:45	Dai (T1)
15:00	Della Latta (T1)
15:15	Di Gregorio (T1)
15:45	Coffee break & poster
16:30	Flash communication
18:30	Welcome Party

Time Tuesday 05	
Chair	<i>Peddís</i>
9:45	Pelosi (T1)
10:00	Piscino (T1)
10:15	Pratolongo (T1)
10:30	Coffee break & poster
11:30	Punis (T1)
11:45	Salemi (T1)
12:00	Livolsi (T3)
12:15	Malannata (T3)
12:30	Marazzi (T3)
12:45	Mulas (T3)
13:00	Light lunch
Chair	<i>Gianotti</i>
15:15	Muñoz García (T3)
15:30	Bisio (K-T1)
16:00	Murgia (T3)
16:15	Coffee break & poster
18:00	Public engagement

Time Wednesday 06	
Chair	<i>Gentili</i>
9:45	Etzi (T5)
10:00	De Leo (T2)
10:15	Piacenza (T2)
10:30	Coffee break & poster
11:30	Condorelli (K-T5)
12:00	Ghibaudo (T5)
12:15	Gatto (T2)
12:30	Honorio Franco (T2)
12:45	Lazzarini (T5)
13:00	Light lunch
Chair	<i>Damin</i>
14:30	Malferrari (T2)
14:45	Mangiacapre (T2)
15:00	Massardo (T2)
15:15	Mastrogiacomo (T2)
16:30	Coffee break & poster
20:00	Social dinner

Time Thursday 07	
Chair	<i>Erba</i>
9:45	Maurelli (T2)
10:00	Gentili (K-T2)
10:30	Coffee break & poster
11:30	Tortorella (T2)
11:45	Tuccitto (T2)
12:00	Varsalona (T2)
12:15	Ruffino (T2)
12:30	Selli (K-T5)
13:00	Light lunch
Chair	<i>Scarano</i>
14:30	Gomez Maya (T2)
14:45	Venanzi (T2)
15:00	Kakkar (T6)
15:15	Vaghi (T4)
15:30	Coffee break & poster
17:00	Maccarino (T6)
17:15	Mancini (T6)

ARISTOTELE

Encapsulation of Fludioxonil in lipid-based nanocarriers for the treatment of fungal diseases in agriculture: preliminary results

Vincenzo De Leo¹, Angelo Agnusdei², Anna Maria Maurelli¹, Donato Gerin², Francesco Faretra², Stefania Pollastro², Lucia Catucci¹

¹*Department of Chemistry, University of Bari Aldo Moro, Via Orabona 4, 70126 Bari, Italy*

²*Department of Soil, Plant and Food Sciences, University of Bari Aldo Moro, Via Orabona 4, 70126 Bari, Italy*
vincenzo.deleo@uniba.it

The aim of this work was to realize lipid nanocarriers (liposomes) loaded with the phytopharmaceutical Fludioxonil (FLUD), for the containment of fungal diseases in agriculture. The application of nanostructured lipid carriers in agriculture finds its motivation in the need to overcome the problems associated with the traditional use of pesticides, such as poor bioavailability, easy degradation, and excessive dispersion in the environment. The research was conducted within the *Sos&Bio_for_One Health* project of the University of Bari.

Two methods were compared for the preparation of liposomes: the Micelle-Vesicle Transition (MVT) method and the extrusion method. Furthermore, three types of vesicles were compared that differed in composition: (I) Plain vesicles, composed of soy phosphatidylcholine and cholesterol; (II) PEG-coated vesicles, with an additional polyethylene glycol coating; and (III) Cationic vesicles, containing a cationic component capable of modifying the surface charge of liposomes (DDAB). The operating parameters, with particular regard to the total amount of lipids and the lipid/FLUD ratio, have been optimized to obtain stable, nanometric-sized vesicles with good Encapsulation Yields (EE%) and Drug Loading (DL%). In particular, through the MVT method, small unilamellar vesicles (SUVs) having a variable mean diameter in the range 80 nm – 150 nm and EE% higher than 78% were easily obtained. The extruded samples yielded mean diameter sizes between 93 nm and 150 nm, with EE% greater than 90%. With both methods the Zeta potential values measured were, in line with expectations, moderately negative for the Plain vesicles and PEG-coated samples and moderately positive for the Cationic vesicles. Subsequently, *in vitro* release tests of the systems loaded with FLUD were performed. A fairly slow release was verified in the early stages, to then reach higher values and remain constant in the following hours. In particular, for the Plain vesicles a plateau was reached at 96.6% after about five hours, compared to 73.4% for the PEG-Coated vesicles and 46% for the Cationic vesicles. Finally, preliminary tests of biological activity against the *Botrytis cinerea* fungus have been carried out. Conidial germination test, inhibition of germ-tube growth and radial growth inhibition test were conducted. In general, FLUD delivered via liposomes showed slightly better performance than free FLUD only at the lowest tested concentrations (0.1-0.3 µg/ml), while it showed similar performance to free drug at high concentrations (1 µg/ml). For intermediate concentration values, free FLUD showed better performance than the liposomal one. Further investigations are underway to evaluate the biological response of FLUD-loaded vesicles by adapting the experimental protocols to the realized systems.

[1] Sostanze naturali, microrganismi e nanocarrier bio-compatibili per lo sviluppo di azioni sostenibili con un approccio "One-Health" e la valorizzazione della biodiversità (*Sos&Bio_for_One Health*)