

From Intermolecular Forces to Frontiers in Nanoscience and Nanomedicine

20-22 January 2016

Adriatico Guesthouse, ICTP, Trieste, Italy

The aim of the workshop is to celebrate the scientific career of Giacinto Scoles in the fields of Physical Chemistry, Biophysics, Nanotechnology, and Nanomedicine, and to recognize his two souls (experimental and theoretical). The invited speakers are representatives of the close relatives (siblings, children and grandchildren) within Giacinto's large scientific family. We hope that the audience will be able to recognize in their presentation of the state-of-the-art in one of the above fields a piece of Giacinto's mind and spirit.

Tentative Programme:

Wednesday, 20 January 2016

9:30-10:00 **Welcome Ceremony (chair L. Casalis)**

10:00-10:50 Inaugural Talk Y.T. LEE (Academia Sinica Taiwan) (Nobel Chemistry 1986)
Half a Century's Comradeship

10:50-11:10 Coffee break

BIOPHYSICS (chair F. Biscarini - Unimore)

11:10-11:55 S. GUSTINCICH (Sissa)
TBA

11:55-12:40 M. HAVENITH (UniBochum)
TBA

12:40-14:00 Lunch

BIOMATERIALS (chair M. Canepa – Università di Genova)

14:00-14:45 M. PRATO (UniTrieste)
Opportunities and Challenges for Carbon-Based Nanomaterials

14:45-15:30 S. KROL (IFOM Milano)
Nanoparticles - two faces of a coin

15:30-16:15 M. MORGANTE (Uniud)
TBA

16:15-16:30 Coffee break

CELLULAR MEDICINE (Chair M. Confalonieri – Cattinara Hospital)

16:30-17:15 A. LAIO (Sissa)
Fast and reliable taxonomy of microbiotas by Density Peak clustering

17:15-18:00 N. ELVASSORE (Unipadova)

3D cell cultures

18:00-18:45 D. CESSELLI (Uniud)

Cancer: the role of microenvironment

18:45-19:30 F. DEL BEN (CRO Aviano)

A metabolism-based approach for Circulating Tumor Cells detection

19:30-21:00 Reception with Poster Session

Thursday, 21 January 2016

BIOMATERIALS (Chair C.A. Beltrami - Uniud)

9:15 -10:00 F. STELLACCI (EPFL Switzerland)

On the interaction of nanoparticles with viruses

10:00-10:45 L. FRUK (Cambridge University)

Biofunctionalized Nanotools for Hybrid Materials Design

10:45-11:00 Coffee break

SIMULATIONS I (Chair G. P. Brivio – Unimi Bicocca)

11:00-11:45 R. ROUSSEAU (PNNL Richland Wash. USA)

Theoretical studies of programs in catalysis

11:45-12:30 E. TOSATTI (Sissa)

TBA

12:30-14:00 Lunch

BIOMATERIALS (Chair T. Da Ros - Unitrieste)

14:00-14:45 F. SCHREIBER (Tuebingen University)

Interactions of Proteins Tailored by Multivalent Ions

14:45-15:30 A. MORGANTE (Director of IOM-CNR)

Charge transfer processes in organic nano – and hetero - structures

15:30-15:45 Coffee break

BIOPHYSICAL CHEMISTRY (Chair S. Onesti)

15:45-16:30 M. CASTRONOVO (Uniud)

Controllable restriction enzyme behaviors over 3D, 2D and 1D DNA nanostructures

16:30-17:15 A. DE MARCO (University of Nova Gorica, Vipava)

Molecular recognition: is there a rational approach to select and develop optimal reagents?

17:15-18:30 V. VOGEL (ETH Zurich)

Stretching our imagination: why forces matter

20:00 DINNER--- With speeches by Y.T. LEE, E. TOSATTI, A. LEVI

Friday, 22 January 2016

WATER (Chair Nino Bracco - Unigenova)

9:15-10:00 R. CAR (Princeton University, Chemistry and Physics)

DFT plus Van der Waals simulations of water properties

10:00-10:45 O. AKIN-OJO (Abuja University of Science and Technology)

Mini Water Festival: The Rise and Fall and Rise of Water Models

10:45-11:00 Coffee break

ENERGY (Chair M. Prato - Unitrieste)

11:00-11:45 M. FERMEGLIA (Unitrieste)

Materials by design: multiscale molecular modeling of nanostructured materials

11:45-12:30 F.TOMA (Lawrence Berkeley Laboratory)

Towards Viable Artificial Photosynthetic Devices

12:30-13:30 Lunch

SIMULATIONS II (Chair S. Scandolo - ICTP)

13:30-14:15 M. PARRINELLO (ETH Zurich – Lugano campus)

Variational enhanced sampling

14:15-15:00 A. SELLONI (Princeton University, Chemistry)

Theoretical studies of materials

15:00-15:45 S. FORTUNA (UniUD)

Computationally engineered binders for protein recognition

15:45 -16:00 Coffee break

LASERS (Chair F. Parmigiani – Elettra Sincrotrone)

16:00-16:45 F. STIENKEMEIER (UniFriburg i. B., Physics)

Beamer – Probing Water Droplets and Functional Molecular Structures

16:45-17:30 D. COJOC (IOM-CNR Basovizza, TS)

Single cell probing by optical tweezers

17:30-18:00 Concluding Remarks: G. SCOLES con I dieci cavalieri dell' apocalisse udinese

