National Conference of ICSC Spoke 7
MATERIALS & MOLECULAR SCIENCES

Event Dates: May 12-14, 2025
Venue: Budinich Lecture Hall, ICTP, Strada Costiera, 11 - I-34151 Trieste, Italy
Organizing Committee: I. Carnimeo, A. Marrazzo, F. Santoro, A. Ruini, F. Dolcini, A. Fortunelli
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ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

Monday May 12

13:30 Registration
14:30 Welcome by Sandro Scandolo (ICTP) & Introduction and overview about the National Centre (Stefano Fabris, Stefano Baroni)
14:45 Keynote: Piotr Lusczek *Accelerating High Performance Computing, Programming Models/Languages & Performance Engineering* (Research Director at the University of Tennessee, MIT Lincoln Lab)
15:25 Pietro Delugas (SISSA) *Quantum ESPRESSO and HPC, history, status, and outlook*
15:45 Fulvio Paleari (CNR-NANO) *Efficient first-principles calculations of exciton-phonon coupling for theoretical spectroscopy and excited-state dynamics in crystals with YAMBO*
16:05 Coffee break (30')
16:35 Giacomo Ambrogio (UniTO) *Large-scale DFT calculations of materials on CPU/GPU architectures with CRYSTAL*
16:55 Daniele Rapetti (SISSA) *Bringing PLUMED to the GPU: implementing a flexible parallelization interface for a community developed code*
17:15 Tommaso Nottoli (UniPI) *An Efficient Implementation of Coupled Cluster with Cholesky Decomposition and Point-Group Symmetry*
17:35 Lucian Constantin (CNR-IMM) *DFT developments: 1) Correlation Energy Functionals from Adiabatic-Connection formalism and 2) Dynamical Kinetic Energy Functionals for Plasmonics*

Poster session (with refreshments)

Tuesday May 13

09:00 Keynote: Jan Gerit Brandenburg (Director for Digital Chemistry, Merck) *Scaling Digital Chemistry at Merck: Synergies from Academia to tackle industry challenges*
09:40 Bernardino Tirri & Giacomo Melani (ENI) *Industrial HPC for Material Science: Eni and Research Centers* Advancing Towards High-Throughput Screening
10:00 Giacomo Melani (CNR-Pisa & ENI) *Machine learning-Accelerated DFT Sampling of Dynamical Processes in Catalysis and Materials Science*
10:20 Coffee break (30')
10:50 Stefano Monteduro (Granarolo), Righero Giuseppe (Lavazza), Giorgia Brancolini (CNR-NANO), Domenico Marson (UniTS) *TBA*
11:30 Alessandro Nanni (Agromateriae/Tampieri) *Agro-industrial Waste Valorization through Computational Design*
11:50 Roundtable (Elisa Molinari, Nicola Marzari, Jan Gerit Brandenburg, Cristina Africh, Alessia D'Orazio)
12:50 Lunch
14:40 Keynote: Nicola Marzari (EPFL and PSI, Director NCCR MARVEL) *The shape of things to come*
15:20 Omar Abou El Kheir (UniMIB) *Machine learning interatomic potential of phase change materials for electronic memories and neuromorphic computing*
15:40 Davide Bidoggia (UniTS) *Structural phase transitions in monolayer transition-metal dichalcogenides with a neural-network interatomic potential*
16:00 Coffee break (30')
16:30 Andrea Maslov (Leonardo S.p.A.) *Exploring innovation: Leonardo's R&D framework and the development of the ASGARD project*
16:50 Emanuela Zaccarelli (CNR-ISC Roma) *TBA*
17:10 Matteo Signorile (UniTO) *Enhancing materials characterization with computational tools*
17:30 Alessio Bartocci (UniTN) *How protein-ligand interactions can modulate protein functions: insights from molecular dynamics simulations*
17:50 Bijoy Nharangatt (UniFI) *Unveiling the Origin of the Unique Magnetism in bulk and monolayer 1T-CrX_2 via Ab Initio Insights*

Poster session (with refreshments)

Wednesday May 14

09:00 Nadia Rega (Full professor in Physical Chemistry, UniNA) *Insights from vibrational dynamics on photorelaxation and non-linear optical spectroscopy techniques*
09:40 Gloria Mazzone (UniCAL) *Computational assessment of novel ruthenium complexes as photherapeutic agents*
10:00 Samuele Giannini (CNR-ICCOM) *Toward an Accurate Description of the Nature and Quantum Dynamics of Electronic Excitations in Extended, Vibrationally Noisy, Molecular Aggregates*
10:20 Leonardo Belpassi (CNR-SCITEC Perugia) *Fully relativistic Dirac-Kohn-Sham calculations for molecules in a complex environment: one step towards the exascale computing*
10:40 Coffee break (30')
11:10 Michele Re Fiorentin (PoliTO) *Computer aided design of bimetallic compound surfaces for CO_2 electroreduction*
11:30 Daniele Perilli (UniMIB) *Engineering Graphene via Doping: Tuning Its Properties for Molecular Gas Interactions*
11:50 Federica Lauria (UniTO) *Solvent simulation strategies in organic chemistry*
12:10 Ignazio Vacante (CNR-IMM Catania) *Bridging length and time scales for materials properties and industrial process simulations*
12:30 Samuele Giuli (SISSA) *Effective and efficient ways to model strong correlation effects in real materials*
12:50 Concluding remarks + QEF poster award
13:00 Lunch

Spoke Assembly

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