The van der Waals – London Discussions

Perugia, October 12 – 14th 2026

Program

Plenary Lectures

Alexander Tkatchenko (University of Luxembourg, LU)
Jean-Pierre Djukic (CNRS, FR)
Martin P. Head-Gordon (University of California, Berkeley, US)
Sereina Riniker (ETH Zurich, CH)

Invited Speakers

Alexander A. Auer (Max-Planck-Institut fur Kohlenforschung, DE)
Almaz Khabibrakhmanov (University of Luxembourg, LU)
Ángel Martín Pendás (University of Oviedo, ES)
Christoph Riplinger (FACCTs GmbH, DE)
Christian Wagner (FRZ-Jülich, DE)
Edoardo Mosconi (CNR-SCITEC, IT)
Enrico Ronca (University of Perugia, IT)
Ganna Gryn'ova (University of Birmingham, UK)
Michele Pavone (University of Napoli, IT)
Róbert Izsák (Riverlane Research Ltd, UK)

Scientific Committee

Giovanni Bistoni (University of Perugia, IT)
Alexandre Tkatchenko (University of Luxembourg, LU)
Jean-Pierre Djukic (University of Strasbourg, FR)

Organizing Committee

Beatrice Bizzarri (F&B Events SRL, IT)
Giulia Marra (CNR-SCITEC, IT)
Maria Letizia Merlini (University of Perugia, IT)

The van der Waals – London Discussions

Perugia, October 12 – 14th 2026

Day 1 - Monday, October 12th 2026	
12:30 – 14:00	**Welcome Coffee**
14:00 – 14:15	***Opening Words*** **by prof. Giovanni Bistoni, University of Perugia, Italy**
Session "London Dispersion: From Fundamentals to Applications" Chairperson: Giovanni Bistoni	
14:15 – 14:55 **PL**	**Alexandre Tkatchenko** *"How atoms interact within molecules beyond covalent bonds"* University of Luxembourg, Luxembourg
14:55 – 15:10 **OC**	**Thomas Froitzheim** *"DFT-D5: a next-generation dispersion correction for the elements H to Lr (Z=1-103)"* University of Bonn, Germany
15:10 – 15:25 **OC**	**Gianluca Regni** *"Bridging spatial and atomic perspectives in the quantitative analysis of London dispersion"* University of Perugia, Italy
15:25 – 15:40 **OC**	**Ciro Guido** *"How dispersion interactions at the excited state can tune photochromism of embedded chromophores"* University of Piemonte Orientale, Italy
15:40 – 15:55 **OC**	**Gabriel José Gil Pérez** *"Frequency-dependent open quantum system modelling of dispersion solute-solvent interactions"* University of Piemonte Orientale, Italy
15:55 – 16:30	**Coffee Break**

Session "Chemical Bonding, Interactions, and Reactivity" **Chairperson: Giovanni Bistoni**	
16:30 – 17:00 **IS**	**Ángel Martín Pendás** *"On differential delocalization of the electrons of a Lewis pair. The case of dative and ionic bonds"* University of Oviedo, Spain
17:00 – 17:15 **OC**	**Martina Colucci** *"Coupled-cluster analysis of intramolecular and intermolecular interactions in complex systems: from weak interactions to covalent bonds"* University of Perugia, Italy
17:15 – 17:30 **OC**	**Sofia Lerda** *"Non-covalent interactions in confined asymmetric catalysis"* University of Perugia, Italy
17:30 – 17:45 **OC**	**Daniele Bondi** *"Energy transfer catalysts for fumarate to maleate isomerization: a computational investigation"* University of Bologna, Italy
17:45 – 17:50 **PP**	**Monia Zarhouni** *"The generalized fragment-resolved activation strain model"* University of Perugia, Italy
17:50 – 17:55 **PP**	**Gerard Comas Vilà** *"Extracting chemical concepts with effective fragment orbitals"* University of Perugia, Italy
17:55 – 19:30	**Welcome Aperitivo**

Day 2 - Tuesday, October 13th 2026

09:00 – 09:10	**Workshop Desk**
Session title: "Modeling Molecular Interactions Across Scales" Chairperson: Paola Belanzoni	
09:10 – 09:50 **PL**	**Sereina Riniker** *"Multiscale neural network potential for the simulation of protein dynamics and enzymatic reactions"* ETH Zurich, Switzerland
09:50 – 10:20 **IS**	**Christoph Riplinger** *"Noncovalent interactions from coupled cluster to hundreds of millions of atoms"* FACCTs, Germany
10:20 – 10:35 **OC**	**Lorenzo Baldinelli** *"Structure–property relationships in host–guest systems: tailoring workflows to capture noncovalent interactions"* CNR-SCITEC, Italy
10:35 – 10:40 **PP**	**Malika Bourjila** *"Side-chain effect on allowed and forbidden regions in ramachandran plot of dipeptide backbone conformations: an exploratory study by using multi niche crowding genetic algorithm"* Faculté des sciences, Morocco
10:40 – 11:10	**Coffee Break**

Session title "Data-Driven Methods for Molecular and Materials Modelling"
Chairperson: Enrico Ronca

11:10 – 11:40	**IS**	**Ganna Gryn'ova** *"Two-dimensional covalent organic frameworks: from modelling to machine learning"* University of Birmingham, United Kingdom
11:40 – 11:55	**OC**	**Alexander Kanzow** *"The interference index: quantifying and training error cancellation in machine-learned thermodynamic stability predictions"* Georg-August-Universität Göttingen, Germany
11:55 – 12:10	**OC**	**Cesare Boriosi** *"A cluster strategy for predicting reaction energies, using energy-decomposition hyperplanes"* University of Perugia, Italy
12:10 – 12:25	**OC**	**Miguel Gallegos Gonzalez** *"IQARIS: a real-space quantum atlas of the CHONSFPCl chemical space"* University of Luxembourg, Luxembourg
12:25 – 12:40	**OC**	**Emilio Lorini** *"Self-assembly of closed- and open-shell nanographenes from machine-learning molecular dynamics"* University of Florence, Italy
12:40 – 12:45	**PP**	**Carlos Roberto Jacinto** *"Extrapolated non-covalent energies in DFT at a fraction of the cost"* University of Perugia, Italy
12:45 – 14:00		**Light Lunch**

Session "Electron Density and Charge Redistribution in Noncovalent Interactions" Chairperson: Leonardo Belpassi	
14:00 – 14:40 **PL**	**Martin P. Head-Gordon** *"Charge flow in intermolecular interactions and its energetic consequences"* University of California, Berkeley, United States
14:40 – 15:10 **IS**	**Almaz Khabibrakhmanov** *"Beyond an energy correction: how van der Waals interactions reshape the electron density"* University of Luxembourg, Luxembourg
15:10 – 15:25 **OC**	**Bartosz Tyrcha** *"Electron density changes in noncovalent interactions within SAPT framework"* Nicolaus Copernicus University in Toruń, Poland
15:25 – 15:40 **OC**	**Humahuti Dihingia** *"Accurate intermolecular induction without over-polarization"* Nicolaus Copernicus University in Toruń, Poland
15:40 – 15:55 **OC**	**Yann Cornaton** *"Unveiling noncovalent interaction patterns along reaction paths using density-based descriptors"* University of Strasbourg, France
15:55 – 16:30	**Coffee Break**
Session "Quantum Technologies for Molecular Interactions" Chairperson: Leonardo Belpassi	
16:30 – 17:00 **IS**	**Enrico Ronca** *"Manipulating weak interactions by quantum fields"* University of Perugia, Italy

17:00 – 17:30 **IS**	**<u>Róbert Izsák</u>** *"Quantum computing for chemistry and material science: trends and recent progress"* Riverlane Research Ltd, United Kingdom
17:30 – 17:45 **OC**	**<u>Diego Sorbelli</u>** *"Probing static and dynamic co-crystal host effects on the spin-optical interface of CR(IV) molecular qubits"* University of Perugia, Italy
17:45 – 18:00 **OC**	**<u>Carlo Gaggioli</u>** *"Modelling singlet oxygen generation on metal organic frameworks with trapped ion quantum computers"* Quantinuum Ltd, United Kingdom
18:00 – 19:45	***Free time***
19:45 – 21:30	**Social Dinner**

Day 3 - Wednesday, October 14th 2026

08:50 – 09:00	**Workshop Desk**
Session title: "Measuring and Modelling Noncovalent Interactions" Chairperson: Edoardo Mosconi	
09:00 – 09:40 **PL**	**Jean-Pierre Djukic** *"Isotherm titration calorimetry in noncovalent interaction research"* CNRS, France
09:40 – 10:10 **IS**	**Christian Wagner** *"Measuring molecule-metal van der Waals interactions in a scanning probe microscope"* FRZ-Jülich, Germany
10:10 – 10:25 **OC**	**Marco Paolantoni** *"Hydration water by vibrational spectroscopy"* University of Perugia, Italy
10:25 – 10:40 **OC**	**Mike Pauls** *"Efficient simulation of induced circular dichroism in noncovalent complexes"* RWTH Aachen University, Germany
10:40 – 10:45 **PP**	**Saskia Krug** *"Quantifying anisole dimer interactions in solution with a molecular balance"* Justus-Liebig-Universität Giessen, Germany
10:45 – 10:50 **PP**	**Mario Ezequiel Perez** *"Ab-initio calculations of mass spectra"* University of Perugia, Italy
10:50 – 11:20	**Coffee Break**

Session title: "Computational Materials for Energy Conversion and Photochemistry"
Chairperson: Luca Gregori

11:20 – 11:50	**IS**	**Michele Pavone** *"Charge transport across heterogeneous functional interfaces: applications to energy conversion devices"* University of Napoli, Italy
11:50 – 12:20	**IS**	**Edoardo Mosconi** *"Computational modeling of new generation materials for photovoltaics and photocatalysis"* CNR-SCITEC, Italy
12:20 – 12:35	**OC**	**Emanuele Priola** *"Structure–property relationships in low-dimensional triphenylsulfonium based organometal lead halide perovskitoids"* University of Turin, Italy
12:35 – 12:50	**OC**	**Chiara Corapi** *"Modelling ground and excited state properties of copper-halide based systems featuring elusive interatomic interactions"* University of Bologna, Italy
12:50 – 12:55	**PP**	**Amanda Covarelli** *"Additives in metal-halide perovskite solar cells: a computational study"* University of Perugia, Italy
12:55 – 13:00	**PP**	**Margarita Shepelenko** *"Frozen by light: Laser-induced ice nucleation unveiled via a DFT snapshot"* Weizmann Institute of Science, Israel
13:00 – 14:30		**Light Lunch**

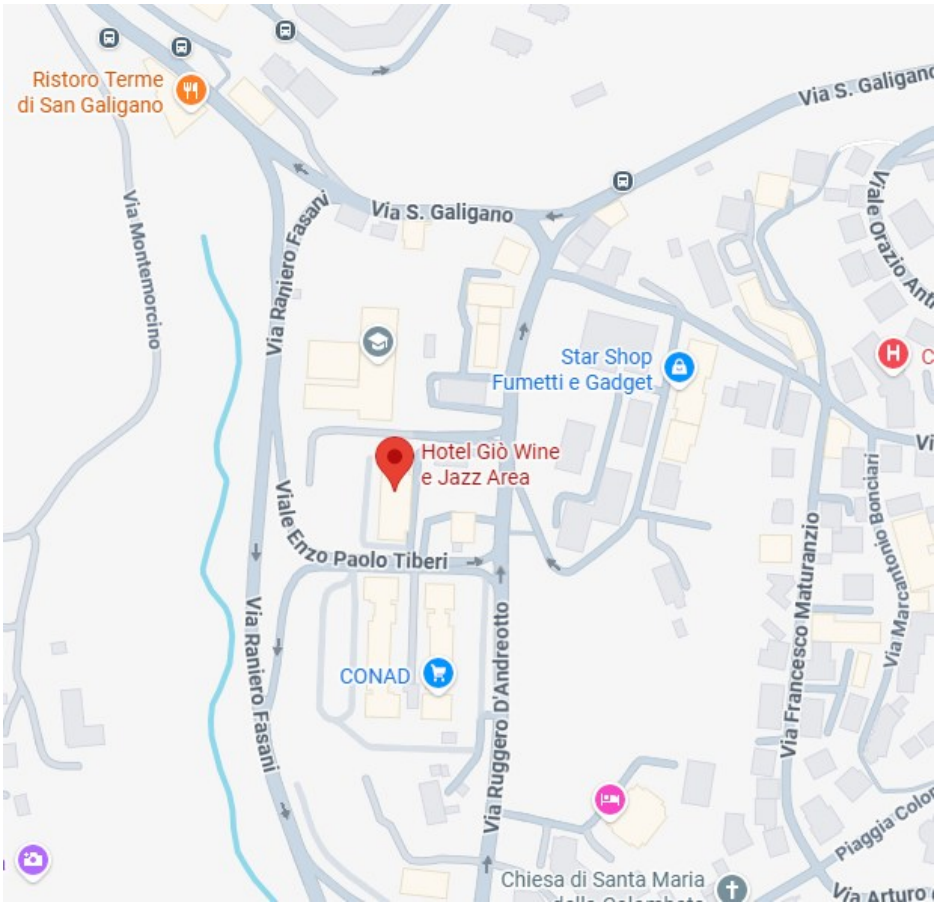
Session title: "Computational Perspectives on Weak and Noncovalent Interactions"
Chairperson: Diego Sorbelli

14:30 – 15:00 **IS**	**Alexander Auer** *"Intramolecular interactions of heavy pnictogen compounds"* Max-Planck-Institut fur Kohlenforschung, Germany
15:00 – 15:15 **OC**	**Guillaume Thiam** *"An efficient DFT/DLPNO-CCSD(T) strategy for weakly bound anions beyond DFT: local coupled-cluster corrections for weakly bound anions"* University of Perugia, Italy
15:15 – 15:30 **OC**	**Paolo Nicolini** *"Simple corrections for directional hydrogen bonding"* Institute of Physics of the Czech Academy of Sciences, Czechia
15:30 – 15:45 **OC**	**Mattia Raimondo** *"Composite DFT methods for weakly bounded solids: from molecular crystals to organic minerals"* University of Turin, Italy
15:45 – 16:00 **OC**	**Sergio Suárez Dou** *"Sampling and spectroscopic features of noncovalent interactions with machine-learned force fields"* University of Luxembourg, Luxembourg
16:00 – 16:15	**Awards**
16:15 – 16:45	**Closing and Remarks**

Venue

The workshop will be held at the Hotel Giò Wine & Jazz Area in Perugia, a distinctive venue combining contemporary comfort with a unique jazz-inspired atmosphere. Located in a convenient position close to Perugia's historic city centre, the hotel offers well-equipped spaces and dedicated facilities for conferences, meetings and scientific events. Its welcoming environment, together with its distinctive character and excellent hospitality, will provide an ideal setting for the vdW/L 2026 workshop.

[Hotel Giò Wine & Jazz Area – Via Ruggero D'Andreotto 19, 16124 Perugia (PG)]



Social Program

Welcome Coffee

Monday, October 12th, 2026 - 12:30 PM

Hotel Giò Wine & Jazz Area

Via Ruggero D'Andreotto 19, 16124 Perugia (PG)

Welcome Aperitivo

Monday, October 12th, 2026 - 5:55 PM

Hotel Giò Wine & Jazz Area

Via Ruggero D'Andreotto 19, 16124 Perugia (PG)

Social Dinner

Tuesday, October 13th, 2026 - 7:45 PM

Hotel Giò Wine & Jazz Area

Via Ruggero D'Andreotto 19, 16124 Perugia (PG)

Brunches & Coffee Breaks

Every Day

Hotel Giò Wine & Jazz Area

Via Ruggero D'Andreotto 19, 16124 Perugia (PG)