DAY 1: MONDAY 9 SEPTEMBER 2019				
12:00-13:30	**REGISTRATION**			
13:30-13:45	**WELCOME and OPENING**			
13:45-14:35	**Room: LAUSANNE** Chairperson: Christoph Dellago **Hardy Gross (***Plenary Speaker)* The Hebrew University of Jerusalem, Israel **Potential Energy Surfaces and Berry Phases from the Exact Factorization: A Predictive First-Principles Approach to Non-Adiabatic Dynamics**			
	Room: ORSAY	**Room: BLARICUM**	**Room: LAUSANNE**	**Room: LYON**
	First Principle Materials Science and High Throughput Chairperson: Leon Petit	**Statistical Physics and Physical Chemistry** Chairperson: Godehard Sutmann	**Algorithm Development and Mathematical Foundations** Chairperson: Carsten Hartmann	**Quantum and Ab-Initio Dynamics** Chairperson: David Coker
14:45-15:15	**Luca Ghiringhelli** Fritz Haber Institute of the Max Planck Society, Berlin, Germany **Big Data and Artificial Intelligence in Materials Science: When The New Science Is in The Outliers**	**Angelos Michaelides (***Invited Speaker***)** University College London, United Kingdom **Interfacial Water: from Atmospheric Ice Nucleation to Nano-Confinement**	**Mark Tuckerman** (*Invited Speaker*) New York University, USA **Molecular Simulation and Machine Learning as Routes to Exploring Structure and Phase Behavior in Atomic and Molecular Crystals**	**Roi Baer** (*Invited Speaker*) The Hebrew University of Jerusalem, Israel **Unraveling Nonequilibrium Dynamics of Non-Interacting Electrons in Open Systems**
15:15-15:45	**Hannes Jonsson** (*Invited Speaker*) University of Iceland, Reykjavík **Self-interaction corrected functional calculations of molecules and solids**	**Lyderic Bocquet** (*Invited Speaker*) École Normale Supérieure (ENS), Paris, France **Mechano-Sensitive Ion Conduction in Nanochannels**	**Benedict Leimkhuler (***Invited Speaker***)** University of Edinburgh, United Kingdom **Exploring Complex Landscapes: from Molecular Dynamics to Neural Networks**	**Aaron Kelly** (*Invited Speaker*) Dalhousie University, Canada **Nonequilibrium Charge and Energy Transport**
15:45-16:05	**Ralph Gebauer** (*Contributed Talk*) International Centre for Theoretical Physics, Trieste, Italy **Water Splitting on Hematite Surfaces: Insights from Density-Functional Theory**	**Alberto Giacomello** (*Contributed Talk*) University of Rome 'La Sapienza', Italy **Perpetual Superhydrophobicity: Drying from the Nanoscale to the Macroscale**	**Pietro Faccioli** (*Contributed Talk*) University of Trento, Italy **All-Atom Simulation of Protein Folding and Direct Validation Against Time-Resolved Spectroscopy Experiments**	**Lidice Cruz Rodríguez** (*Contributed Talk*) Research Institute on Complex Atomic and Molecular Systems, Toulouse, France **Trajectory-Based Method for the Study of Ultrafast Quantum Dynamics.**
16:05-16:35	**COFFEE BREAK**			

	Room: ORSAY	Room: BLARICUM	Room: LAUSANNE	Room: LYON
	High-Throughput and Big Data	**Statistical Physics and Physical Chemistry**	**Algorithm Development and Mathematical Foundations**	**Soft Matter**
16:35-16:55	**Jutta Rogal** (*Contributed Talk*) Ruhr-University Bochum, Germany **Neural Network-Based Path Collective Variables for Enhanced Sampling of Phase Transformations**	**Felix Höfling** (*Contributed Talk*) Free University of Berlin, Germany **Emergence of Molecular Friction in Liquids: A Memory-Kernel Perspective**	**Erik.E. Santiso** (*Contributed Talk*) North Carolina State University, USA **Modeling Crystal Nucleation with the String Method**	**Gerhard Kahl** (*Contributed Talk*) Vienna University of Technology, Austria **Dendrimer-Like DNAs: Simulation and Experiment**
16:55-17:15	**Daniele Padula** (*Contributed Talk*) Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland **Singlet Fission Molecules among Known Compounds: Finding a Few Needles in a Haystack**	**Céline Merlet** (*Contributed Talk*) CNRS-University of Toulouse, France **Simulation of NMR Spectra for Molecules or Ions Diffusing in Porous Disordered Carbons**	**J. Zhang** (*Contributed Talk*) Peking University, Beijing, China **Learning Clustered Representation for Complex Free Energy Landscapes**	**Jure Dobnikar** (*Contributed Talk*) Chinese Academy of Sciences, Beijing, China University of Cambridge, United Kingdom **Emerging Interactions through Active Alignment**
17:15-17:35	**Max Veit** (*Contributed Talk*) Swiss Federal Institute of Technology (EPFL), Switzerland **Machine Learning Potentials for Molecular Liquids**	**Matteo Ceccarelli** (*Contributed Talk*) University of Cagliari, Italy **Multiscale Modeling of Molecular Diffusive Transport Phenomena: from Microscopic Details to Macroscopic Fluxes**	**Mauricio J. Del Razo** (*Contributed Talk* Free University of Berlin, Germany **Modeling and Simulating Molecular Kinetics as Diffusion Processes with Markovian Switching**	**Silvia Corezzi** (*Contributed Talk*) University of Perugia, Italy **Autocatalytic Patchy Particles**
17:40-18:30	**Room: LAUSANNE**		Chairperson: Michel Mareschal	
	Julia Yeomans (*Plenary Speaker*) University of Oxford, United Kingdom **Topology in Biology?**			

DAY 2: TUESDAY 10 SEPTEMBER 2019

9:00-9:50	**Room: LAUSANNE** Chairperson: Giovanni Ciccotti			
	Giulia Galli (*Plenary Speaker*) University of Chicago, USA **Light-activated matter: from photo-electrochemical cells to optogenetics and quantum information systems**			
9:50-10:30	**COFFEE BREAK**			
	Room: ORSAY	**Room: BLARICUM**	**Room: LAUSANNE**	**Room: LYON**
	Electronic Structure – First Principle Modelling Chairperson: Paul Durham	**Soft Matter** Chairperson: Kurt Kremer	**Biophysics and Biochemistry** Chairperson: Francesco Gervasio	**Statistical Physics and Physical Chemistry** Chairperson: Rodolphe Vuilleumier
10:30-11:00	**Lucia Reining** (*Invited Speaker*) Ecole Polytechnique, Palaiseau, France **Calculation of Electronic Spectra Using Auxiliary Systems and Model Results**	**Marcus Müller** (*Invited Speaker*) Georg-August University, Göttingen, Germany **Structure Formation in Copolymer Materials After Sudden Quenches**	**Erik Lindahl** (*Invited Speaker*) Stockholm University, Sweden **Simulations of Structural Transformations in Ceramide Phases from Fitting Structures to CEMOVIS Image Data**	**Benjamin Rotenberg** (*Invited Speaker*) Sorbonne University, Paris, France **"Use the Force!" Reduced Variance Estimators for Radial Distribution Functions, Generic 3d Densities and (Local) Transport Coefficients**
11:00-11:30	**Kristian Sommer Thygesen** (*Invited Speaker*) Technical University of Denmark, Kongens Lyngby Denmark **Data-Driven Discovery of Novel Two-Dimensional Materials**	**Markus Deserno** (*Invited Speaker*) Carnegie Mellon University, Pittsburgh, USA **The Role of Dynamin Twist in Membrane Fission**	**Ron Elber** (*Invited Speaker*) The University of Texas, Austin, USA **Computer Simulations of Biological Systems: Proteins, RNA and Membranes**	**Kirsten Martens** (*Invited Speaker*) University Grenoble Alpes, France **Modeling Approaches for Soft Glassy Rheology**
11:30-12:00	**Kersti Hermansson** (*Contributed Talk*) Uppsala University, Sweden **OH!**	**Ludovic Berthier** (*Invited Speaker*) University of Montpellier, France **Equilibrium Simulations of Supercooled Liquids Beyond Laboratory Timescales**	**Davide Marenduzzo** (*Invited Speaker*) University of Edinburgh, United Kingdom **Biophysical Principles of Transcription-Driven Chromosome Organisation**	**Nuno Araujo** (*Invited Speaker*) University of Lisbon, Portugal **Self-Folding Kirigami at the Microscale**
12:00-12:20	**Enrico Tapavicza** (*Contributed Talk*) California State University Long Beach, USA **First-Principles Prediction of Vibronic Spectra, Internal Conversion and Wavelength-Dependent Product Quantum Yields**	**Marisol Ripoll** (*Contributed Talk*) Jülich Research Centre, Germany **Phoretic Colloids and Micromachines**	**Marie-Christine Sawley** (*Contributed Talk*) Intel Semiconductor Ag, Zurich, Switzerland **25 Years of Biosimulation**	**Aleksandar Donev** (*Contributed Talk*) Courant Institute, New York University, USA **Fluctuating Hydrodynamics of Electrolytes**
12:20-12:40	**M. V. Ganduglia-Pirovano** (*Contributed Talk*) Institute of Catalysis and Petrochemistry-CSIC, Madrid, Spain **Oxygen-Vacancy Ordering and Dynamics at the Reduced Ceo2(111) Surface and the Entanglement with Polaron Hopping**	**Angelo Rosa** (*Contributed Talk*) International School of Advanced Studies – SISSA, Trieste, Italy **From Chromosome Territories to Ring Polymers: Physical Properties of Untangled Polymers Melts**	**Alberto Pérez de Alba Ortíz** (*Contributed Talk*) University of Amsterdam, The Netherlands **Simultaneous Sampling of Multiple Transition Channels Using Adaptive Paths of Collective Variables**	**Daniel Borgis** (*Contributed Talk*) CNRS-Ecole Normale Supérieure De Paris (ENS), France Maison De La Simulation, Saclay, France **Ion-Induced Long-Range Orientational Correlations in Highly Diluted Electrolytes: What Do Second Harmonic Scattering Experiments Measure?**

12:45-14:15	**LUNCH BREAK**			
14:15-15:05	**Room: LAUSANNE** Chairperson: Berend Smit **Werner Krauth (***Plenary Speaker***)** Ecole Normale Supérieure (ENS), Paris, France **Fast Irreversible Markov Chains in Statistical Physics**			
	Room: ORSAY	**Room: BLARICUM**	**Room: LAUSANNE**	**Room: LYON**
	Materials Modelling Chairperson: Magali Benoit	**Soft Matter** Chairperson: Jean Louis Barrat	**Statistical Physics and Physical Chemistry** Chairperson: Gerhard Kahl	**Biophysics and Biochemistry** Chairperson: Majdi Hochlaf
15:05-15:35	**Mariana Rossi** (*Invited Speaker*) Fritz Haber Institute of the Max Planck Society, Berlin, Germany **Nuclear Quantum Effects in First-Principles Materials Simulations**	**Emanuela Zaccarelli** (*Invited Speaker*) CNR- Institute for Complex Systems, Rome, Italy **In silico Synthesis of Microgels: Structure, Elasticity and Effective Interactions in Bulk and at Liquid-Liquid Interfaces**	**Emanuela Del Gado** (*Invited Speaker*) Georgetown University, Washington DC, USA **The Physics of Smarter and More Sustainable Cements**	**Ralf Everaers (***Invited Speaker*) École Normale Supérieure (ENS), Lyon, France **The Physics of Crumpling and Folding of Untangled Polymers and Chromosomes**
15:35-16:05	**Angel Rubio** (*Invited Speaker*) Max Planck Institute for the Structure and Dynamics of Matter, Mainz, Germany **Quantum-Cavity and Floquet-Engineered New States of Matter from a QEDFT Perspective**	**Marjolein Dijkstra** (*Invited Speaker*) Debye Institute, University of Utrecht, Netherlands **Birth of a Binary Crystal Nucleus of Hard Spheres**	**Gerhard Gompper** (*Invited Speaker*) Jülich Research Centre, Germany **Active Filaments, Membranes, and Cells**	**Marek Cieplak** (*Invited Speaker*) Polish Academy of Science, Warsaw, Poland **Emergence of Knots in Intrinsically Disordered Proteins**
16:05-16:35	**COFFEE BREAK**			
16:35-16:55	**Stefano Mossa** (*Contributed Talk*) Interdisciplinary Research Institute of Grenoble (IRIG), France **Vibrational Excitations and Elastic Response at the Nanoscale: from Disordered Solids to Nanostructures**	**Francisco Vega Reyes** (*Contributed Talk*) University of Extremadura, Spain **Complex Memory in Soft Materials**	**William A. Curtin** (*Contributed Talk*) Swiss Federal Institute of Technology (EPFL), Switzerland **From Density Functional Theory to Strength and Ductility of Complex Metal Alloys**	**A. Marco Saitta** (*Contributed Talk*) Sorbonne University, Paris, France **Prebiotic Chemistry and Origins of Life Studies Through Ab Initio Calculations**
16:55-17:15	**Marcella Iannuzzi** (*Contributed Talk*) University of Zurich, Switzerland **Molecules at the Electrochemical Interface: Understanding Experiments with Simulations**	**Jean Paul Ryckaert** (*Contributed Talk*) University of Brussels, Belgium **Shape, Height Fluctuations and Resisting Force of a Membrane Deformed by an Actin Bundle**	**Kostas Daoulas** (*Contributed Talk*) Max Planck Institute for Polymer Research, Mainz, Germany **Symmetry-Inspired Mesoscopic Models for Studying Partially-Ordered Mesophases of Semiconducting Polymers**	**Birgit Strodel** (*Contributed Talk*) Jülich Research Centre, Germany **Challenges, Advances and Perspectives of Protein Aggregation Simulations**
17:25-18:15	**Room: LAUSANNE** Chairperson: Mauro Ferrario **Gabor Csanyi (***Plenary Speaker)*** University of Cambridge, United Kingdom **Advances in Interatomic Potentials for Materials**			

DAY 3: WEDNESDAY 11 SEPTEMBER 2019

9:00-9:50	**Room: LAUSANNE** Chairperson: Dominic Tildesley			
	Ursula Röthlisberger (*Plenary Speaker*) Swiss Federal Institute of Technology (EPFL), Lausanne, Switzerland **Next-Generation First-Principles Based Molecular Dynamics: From Biological Systems to Materials**			
9:50-10:30	**COFFEE BREAK**			
	Room: ORSAY	**Room: BLARICUM**	**Room: LAUSANNE**	**Room: LYON**
	Electronic Structure – First Principle Modelling Chairperson: Thierry Deutsch	**Statistical Physics** Chairperson: Burkhard Duenweg	**Biophysics and Biochemistry** Chairperson: Vittorio Limongelli	**Physical Chemistry** Chairperson: Florent Calvo
10:30-11:00	**Silvana Botti** (*Invited Speaker*) Friedrich Schiller University, Jena, Germany **Exchange-Correlation Functionals for the Band Structure of Solids: from Bulk Systems to Interfaces and Surfaces**	**Chantal Valeriani** (*Invited Speaker*) Complutense University of Madrid, Spain **The Role Played by Interactions in the Assembly of Active Colloids**	**Ilpo Vattulainen** (*Invited Speaker*) Tampere University of Technology, Finland **Biosimulations in Life Sciences: Coarse-Grained Molecular Simulation Models Are Usually Superb, But When Do We Dare to Use Them?**	**M. Sprik** (*Invited Speaker*) University of Cambridge, United Kingdom **Electromechanics of the Liquid Water-Vapour Interface**
11:00-11:30	**Feliciano Giustino** (*Invited Speaker*) University of Oxford, United Kingdom **Looking Inside a Polaron**	**Matthieu Wyart** (*Invited Speaker*) Swiss Federal Institute of Technology (EPFL), Switzerland **A Jamming Transition Affects Landscape and Generalisation in Deep Learning**	**Modesto Orozco** (*Invited Speaker*) University of Barcelona, Spain **DNA a 10^{10} Multiscale Problem**	**Marialore Sulpizi** (*Invited Speaker*) Johannes Gutemberg University Mainz, Germany **Ionic liquid confined between metallic interfaces: what is the role of image charges?**
11:30-12:00	**Georg Kresse** (*Invited Speaker*) University of Vienna, Austria **Hybrid Perovskites: From the Random Phase Approximation to Machine Learned Potentials**	**Srikanth Sastry** (*Invited Speaker*) Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India **Self Organization and Irreversibility in Cyclically Driven Amorphous Matter**	**Peter Bolhuis** (*Invited Speaker*) University of Amsterdam, Netherlands **Understanding the Dynamical Bottlenecks in Complex Activated (Bio)Molecular Processes**	**Mathieu Salanne** (*Invited Speaker*) Sorbonne University, Paris, France **Electrode Models for Computational Electrochemistry**
12:00-12:20	**Göran Wendin** (*Contributed Talk*) Chalmers University of Technology, Sweden **Calculating Ground State Energy Surfaces for H_2O and HCN with a Quantum Computer**	**Matthias Fuchs** (*Contributed Talk*) University of Konstanz, Germany **Emergence of Long-Ranged Stress and Strain Correlations in Viscoelastic Liquids**	**Elise Dumont** (*Contributed Talk*) École Normale Supérieure (ENS), Lyon, France **Mapping DNA-Photosensitizers Interaction in and Out the Nucleosome**	**Carlo Pierleoni** (*Contributed Talk*) University of L'Aquila, Italy **High Pressure Liquid Hydrogen Across Molecular Dissociation**
12:20-12:40	**Zhao Wang** (*Contributed Talk*) Tu Wien, Vienna, Austria Guangxi University, China **Selective Conduction of Organic Molecules on Free-Standing Graphene and Carbon Nanotubes**	**Giuseppe Foffi** (*Contributed Talk*) University of South Paris, France **Slowing Down Supercooled Liquids by Manipulating their Local Structure**	**Anton Polyansky** (*Contributed Talk*) University of Vienna, Austria **Towards an Atomistic Structure of Phase-Separated Protein Granules**	**Saikat Datta** (*Contributed Talk*) University of Edinburgh, United Kingdom **Nanobubble Nucleation Due to Surface Vibration**
12:45-14:00	**LUNCH BREAK**			

	CECAM 50 CELEBRATION
	Room: LAUSANNE Chairperson: Alessandro Laio
14:00-14:30	**Daan Frenkel** University of Cambridge, United Kingdom **Lecture on CECAM History, Role and Contributions**
14:30-15:45	Berni J. Alder prize ceremony
15:45-16:15	**COFFEE BREAK**
	Room: LAUSANNE Chairperson: Ignacio Pagonabarraga
16:15-18:00	Round table **Silke Biermann** Ecole Polytechnique, Palaiseau, France **Nicola Marzari** Swiss Federal Institute of Technology (EPFL), Switzerland **Elisa Molinari** University of Modena and Reggio Emilia, Italy **Michele Parrinello** ETH Zürich and USI Lugano, Switzerland **Christof Schütte** Zuse Institute Berlin, Germany **Matthias Troyer** One Microsoft Way Redmond, USA **Martin Vetterli** Swiss Federal Institute of Technology (EPFL), Switzerland
19:00-00:00	**CONFERENCE DINNER AT THE OLYMPIC MUSEUM**

DAY 4: THURSDAY 12 SEPTEMBER 2019

9:00-9:50	**Room: LAUSANNE**		Chairperson: Stefano Baroni	
	Ali Alavi (*Plenary Speaker*) Max Planck Institute for Solid State Research, Stuttgart, Germany **Non-Unitary and Stochastic Quantum Chemistry**			
9:50-10:30	**COFFEE BREAK**			
	Room: ORSAY	**Room: BLARICUM**	**Room: LAUSANNE**	**Room: LYON**
	Electronic Structure and Materials Modelling Chairperson: Fabio Affinito	**Statistical Physics and Physical Chemistry** Chairperson: Carlo Maria Bertoni	**Biophysics and Biochemistry** Chairperson: Donal Mackernan	**Physical Chemistry** Chairperson: Matej Praprotnik
10:30-11:00	**Roman Martonak** (*Invited Speaker*) Comenius University, Bratislava, Slovakia **Quantum and Classical Ripples in Graphene**	**Doros Theodorou** (*Invited Speaker*) National Technical University, Athens, Greece **Atomistic and Mesoscopic Simulations of Polymer Melts**	**Simone Meloni** (*Invited Speaker*) University of Ferrara, Italy **Multiscale Simulations of Nanofluidic Porous Systems for Energy Applications**	**Michele Ceriotti** (*Invited Speaker*) Swiss Federal Institute of Technology (EPFL), Switzerland **Machine Learning for Atomic and Molecular Simulations**
11:00-11:30	**Mauro Ferrario** (*Contributed Talk*) University of Modena and Reggio Emilia, Modena, Italy **Monitoring Water Splitting at Graphene Edges: Insights Into the Effects of Humidity on the Lubricity of Graphitic Materials**	**Francesco Mauri** (*Invited Speaker*) University of Rome La Sapienza, Italy **Unified Theory of Thermal Transport in Crystalline Solids and Glasses**	**Ryoichi Yamamoto** (*Invited Speaker*) University of Kyoto, Japan **Impact of Wall Constraint on the Dynamics of Self-Propelled Particles**	**Tanja Schilling** (*Invited Speaker*) University of Freiburg, Germany **Coarse-Graining Out of Equilbrium**
11:30-11:50	**Mauro Causa** (*Contributed Talk*) University of Naples Federico II, Italy **The Maximum Probability Domains (MPD) As a Powerful Tools for Analysing Electronic Structures**	**Stephen J. Cox** (*Contributed Talk*) University of Cambridge, United Kingdom **Stabilization of Agi's Polar Surfaces by the Aqueous Environment, and its Implications for Ice Formation**	**Barak Hirshberg** (*Contributed Talk*) Swiss Federal Institute of Technology (ETHZ), Switzerland **Path Integral Molecular Dynamics for Cold Bosons**	**Grisell Diaz Leines** (*Contributed Talk*) Ruhr University, Bochum, Germany **Maximum Likelihood Analysis of Reaction Coordinates during Crystal Nucleation in N_i**
11:50-12:10	**Tatsuhiko Ohto** (*Contributed Talk*) Osaka University, Japan **Accessing the Accuracy of Density Functional Theory through Structure and Dynamics of the Water−Air Interface**	**Guido Roma** (*Contributed Talk*) University of Paris-Saclay, France **Oxidation Products of Polyethylene and their Optical Signatures**	**Dennis R. Salahub** (*Contributed Talk*) University of Calgary, Canada **Towards Free-Energy Profiles for Nano-Catalyzed Chemical Reactions in Complex Environments**	**Robinson Cortes Huerto** (*Contributed Talk*) Max Planck Institute for Polymer Research, Mainz, Germany **Open Boundaries in Hamiltonian Adaptive Resolution Simulations: from Grand Canonical to Nonequilibrium Molecular Dynamics**
12:25-13:15	**Room: LAUSANNE**		Chairperson: Daan Frenkel	
	Eric Vanden-Eijnden (*Plenary Speaker*) Courant Institute of Mathematical Sciences, New York University, USA **Molecular Dynamics Simulations in the Age of Machine Learning**			
13:20-13:30	**CLOSING CEREMONY**			