Program and Information

CCP2018

XXX IUPAP Conference on Computational Physics
July 29 - August 2, 2018
University of California, Davis, USA

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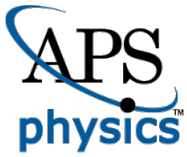
Sponsors of CCP2018



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Welcome to CCP2018

Dear CCP2018 Participants:

It is our pleasure to welcome you to CCP2018, the XXX IUPAP Conference on Computational Physics, at the University of California, Davis. This is the 30th in the CCP conference series continuing the tradition of having the broad international computational physics community convene to present contemporary research results and also to consider the vision of where our field is going.

UC Davis is a comprehensive campus in the University of California system with broad-based programs in the general area of computational physics and related fields. We are consistently ranked as one of the top public universities in the country and the world. In the ten campus UC system, UC Davis is first in physical size, second in total research funding, and third in total student enrollment. At UC Davis we champion the opportunities for learning and success for a broad spectrum of students with rich course offerings in the physical sciences, engineering, biological sciences, agriculture, humanities and arts, and a wide range of professional schools.

UC Davis is located in the California central valley, close to our capital of Sacramento, with easy access by car or public transportation to the San Francisco Bay Area, Napa Valley, Lake Tahoe, Yosemite National Park, and many other venues of historical and cultural interest. We hope you have the time to avail yourself of our beautiful California either before or after the conference.

Enjoy CCP2018 and the broad and interesting program we have worked hard to assemble that we hope will further stimulate your interests in computational physics, provide a venue to present your research, and to collectively help chart the future of computational physics with your colleagues.

Yours sincerely,

Barry M. Klein, *Chair*

Richard T. Scalettar and Warren E. Pickett, *Vice Chairs*

And all the committee members and UC Davis staff that contributed to the organization and implementation of the CCP2018 conference.

A special thanks to Cindy Choi, Giacomo Resta, Teresa Alameda, and Professors Ching Fong and Bernd Hamann for their work on the conference and its program.

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Exhibitors

The following publishers will present exhibits at CCP2018:

- **AIP Publishing**
- **Cambridge University Press**
- **Frontiers**
- **IOP Publishing**

The exhibits are located in the **Conference Center** and will be open **Monday-Thursday**.

Program Overview

	Sun 7/29	Mon 7/30	Tue 7/31	Wed 8/1	Thu 8/2
8am		Registration			
9am		Welcome	Plenary Session	Plenary Session	Plenary Session
		Plenary			
10am		Break			
			Break	Break	Break
11am		Plenary Session	Plenary Session	Plenary Session	Plenary Session
12pm					
		Lunch	Lunch	Lunch	Lunch
1pm					
2pm		Parallel Sessions	Parallel Sessions	Parallel Sessions	Parallel Sessions
3pm					
		Break	Break	Break	Break
4pm	Welcome Reception and Registration	Parallel Sessions	Parallel Sessions	Parallel Sessions	Parallel Sessions
5pm					
6pm			Poster Session	Banquet	
7pm					
8pm					
9pm					

Sunday, July 29

16:00-20:00	**Welcome Reception & Registration** *Location: Buehler Alumni Center*

Monday, July 30

08:00-09:00	**Registration** *(Conference Center, Lobby)*
09:00-09:30	**Welcome** *(Conference Center, Ballroom ABC)* Gary May, *Chancellor of UC Davis* David Landau, *Chair of the C20 Commission of IUPAP* Barry Klein, *Chair of CCP2018*
	Plenary Session *Location: Conference Center, Ballroom ABC* *Chair: Barry Klein*
09:30-10:15	**J. Anthony Tyson**, *University of California, Davis (USA)* Cosmology Data Analysis Opportunities and Challenges in the LSST Sky Survey
10:15-10:45	**Break**
	Plenary Session *Location: Conference Center, Ballroom ABC* *Chair: Barry Klein*
10:45-11:30	**Matthias Troyer**, *Microsoft Quantum (USA); ETH Zurich (Switzerland)* A quantum future for computational physics
11:30-12:15	**Alan Aspuru-Guzik**, *University of Toronto (Canada); Vector Institute (Canada); Zapata Computing (USA)* The era of variational quantum algorithms
12:15-14:00	**Lunch** *(Buehler Alumni Center)*
14:00-15:30	**Parallel Sessions 1** **Machine Learning 1**, *Conference Center, Ballroom A* **Materials 1**, *Conference Center, Ballroom B* **Quantum Many-body 1**, *Conference Center, Ballroom C*
15:30-16:00	**Break**
16:00-18:00	**Parallel Sessions 2** **Machine Learning 2**, *Conference Center, Ballroom A* **Materials 2**, *Conference Center, Ballroom B* **Quantum Many-body 2**, *Conference Center, Ballroom C*

Monday, Parallel Sessions 1

Machine Learning 1	
Location: Conference Center, Ballroom A	**Chair:** Gus Hart
14:00-14:45	**Invited: Ehsan Khatami**, *San Jose State University (USA)* Artificial intelligence: a new tool for the study of quantum many-body systems
14:45-15:00	**Duong-Nguyen Nguyen**, *Japan Advanced Institute of Science and Technology (Japan)* Regression-based clustering for material analysis
15:00-15:15	**Rebecca Lindsey**, *Lawrence Livermore National Laboratory (USA)* ChIMES: Machine-Learned Force Fields for Quantum-Accurate Reactive Simulation
15:15-15:30	**Kipton Barros**, *Los Alamos National Laboratory (USA)* Advances in machine learned potentials for molecular dynamics simulation

Materials 1	
Location: Conference Center, Ballroom B	**Chair:** John Pask
14:00-14:45	**Invited: James Chelikowsky**, *University of Texas (USA)* Extending the Scale with Real-Space Methods for the Electronic Structure Problem
14:45-15:30	**Invited: John Pask**, *Lawrence Livermore National Laboratory (USA)* Discontinuous projection method for large, accurate electronic structure calculations

Quantum Many-body 1	
Location: Conference Center, Ballroom C	**Chair:** Regina Maphanga
14:00-14:45	**Invited: G George Batrouni**, *Université Côte d'Azur, Nice (France); Beijing CSRC (China); MajuLab, CNRS-UNS-NUS-NTU (Singapore)* Langevin QMC algorithm for strongly interacting electron-phonon systems: The phase diagram of two-dimensional model with long range interactions
14:45-15:30	**Invited: Mark B Ritter**, *IBM T.J. Watson Research Center (USA)* Near-Term Quantum Algorithms for Quantum Many-Body Systems

Monday, Parallel Sessions 2

Machine Learning 2	
Location: Conference Center, Ballroom A	**Chair:** Gus Hart
16:00-16:15	**Andrew Horsfield**, *Imperial College London (United Kingdom)* Tight Binding Molecular Dynamics with Electron Open Boundaries
16:15-16:30	**Michael LaCount**, *University of California, Davis (USA)* Comparison and Validation of Recent Exchange-Correlation Functionals for First-Principles Simulations of Water
16:30-16:45	**Tien-Lam Pham**, *JAIST; CMI2-ESICMM, National Institute for Materials Science (Japan)* Learning materials properties from orbital interactions

Materials 2	
Location: Conference Center, Ballroom B	**Chair:** John Pask
16:00-16:15	**Ruizhi Qiu**, *China Academy of Engineering Physics (China)* Energetics of intrinsic point defects in aluminium via orbital-free density functional theory
16:15-16:30	**Zuo-Bing Wu**, *Chinese Academy of Sciences (China)* Multiscale simulation of three-dimensional thin-film lubrication systems
16:30-16:45	**Nir Goldman**, *Lawrence Livermore National Laboratory (USA)* Development of a Multi-center Density Functional Tight Binding Model for Plutonium Surface Hydriding
16:45-17:00	**Alberto Ambrosetti**, *University of Padua (Italy)* Exotic van der Waals interactions in graphene: from ultra-long ranged attraction to ultra-strong screening
17:00-17:15	**Soham Ghosh**, *University of California, Davis (USA)* Spectrum Shifts in H_3S due to Strong Coupling to Phonons
17:15-17:30	**Antia S. Botana**, *Argonne National Laboratory (USA)* Electronic structure of square planar nickelates revisited: relationship to cuprates
17:30-17:45	**Yundi Quan**, *University of California, Davis (USA)* Probing the Origin of High Temperature Superconductivity in H-rich Compounds
17:45-18:00	**Guang-Yu Guo**, *National Taiwan University (Taiwan)* Large anomalous Nernst and spin Nernst effects in noncollinear antiferromagnets Mn3X (X=Sn,Ge,Ga)

Quantum Many-body 2	
Location: Conference Center, Ballroom C	**Chair:** Regina Maphanga
16:00-16:15	**Anthony D. Dutoi**, *University of the Pacific, Stockton (USA)* Excitonic Coupled-cluster Theory for Large-scale Electronic Structure Calculations
16:15-16:30	**H.-Q. Lin**, *Beijing Computational Sciences Research Center (China)* Finite-Temperature Lanczos Method and its Application on Spin Frustrated Systems
16:30-16:45	**Aritra Das**, *Indian Institute of Technology Kanpur (India)* Game of Mixed Entangled States for Social Advantage
16:45-17:00	**Anders Sandvik**, *Boston University (USA)* Random-Singlet Phase in Disordered Two-Dimensional Quantum Magnets
17:00-17:15	**Hui Shao**, *CSRC Beijing; Beijing Normal University (China)* Universality Class and Dangerously Irrelevant Field at Classical and Quantum Phase Transitions
17:15-17:30	**Giacomo Resta**, *University of California, Davis (USA)* Numerical implementation for evaluating vertex corrections to electrical conductivity in multi-band electron systems
17:30-17:45	**Bo Xiao**, *University of California, Davis (USA)* World-line Quantum Monte Carlo Simulation of the Extended Hubbard-Holstein Model with Long-range Electron-Phonon Interaction
17:45-18:00	**Himani Mishra**, *Indian Institute of Information Technology, Allahabad (India)* Study of the influence of structural defects on the optoelectronic properties of two dimensional transition metal dichalcogenides.

Tuesday, July 31

	Plenary Session *Location: Conference Center, Ballroom ABC* *Chair: Warren Pickett*
09:00-09:45	**Defang Duan**, *Jilin University (China)* Hydrogen-rich materials under high pressure: clue and route towards high-temperature superconductors
09:45-10:30	**Matthias Scheffler**, *Fritz-Haber-Insitut der Max-Planck-Gesellschaft (Germany); UC Santa Barbara (USA)* Data-Driven Materials-Science – Rethinking the Pursuit of Understanding
10:30-11:00	**Break**
	Plenary Session *Location: Conference Center, Ballroom ABC* *Chair: Warren Pickett*
11:00-11:45	**Gus Hart**, *Brigham Young University (USA)* Machine Learning and Materials Discovery
11:45-12:30	**Duncan Brown**, *Syracuse University (USA)* GW170817: The Multi-Messenger Observation of a Binary Neutron Star Merger
12:30-14:00	**Lunch** *(Buehler Alumni Center)*
14:00-15:30	**Parallel Sessions 1** **Astrophysics 1**, *Conference Center, Ballroom A* **Materials 3**, *Conference Center, Ballroom B* **Software 1**, *Conference Center, Ballroom C*
15:30-16:00	**Break**
16:00-18:00	**Parallel Sessions 2** **Astrophysics 2**, *Conference Center, Ballroom A* **Materials 4**, *Conference Center, Ballroom B* **Software 2**, *Conference Center, Ballroom C*
18:00-21:00	**Poster Session** *Location: Conference Center* Refreshments will be served at the session

Tuesday, Parallel Sessions 1

Astrophysics 1	
Location: Conference Center, Ballroom A	**Chair:** Duncan Brown
14:00-14:45	**Invited: Peter Nugent**, *Lawrence Berkeley National Laboratory (USA)* The Convergence of HPC and Big Data in Cosmology
14:45-15:30	**Invited: Joshua Dolence**, *Los Alamos National Laboratory (USA)* Simulations of Core-Collapse Supernova Explosions

Materials 3	
Location: Conference Center, Ballroom B	**Chair:** Michelle Johannes
14:00-14:45	**Invited: Eva Zurek**, *University at Buffalo, SUNY (USA)* Computational Discovery of New Materials Under Pressure
14:45-15:30	**Invited: John J. Rehr**, *University of Washington (USA)* Cumulant Green's function approach for excited states, response functions, and thermodynamics

Software 1	
Location: Conference Center, Ballroom C	**Chair:** Jeremy Mason
14:00-14:45	**Invited: Stephen Jordan**, *Microsoft Research; University of Maryland (USA)* Quantum algorithms for simulating quantum field theories
14:45-15:30	**Invited: Nicolas Gauger**, *TU Kaiserslautern (Germany)* Efficient Methodologies for Optimization and Control in Fluid Mechanics

Tuesday, Parallel Sessions 2

Astrophysics 2	
Location: Conference Center, Ballroom A	**Chair:** Duncan Brown
16:00-16:15	**Samiran Das**, *Central Institute of Technology Kokrajhar (India)* Propagation of Dust-Ion Acoustic Solitary Waves in Dusty Plasma with Boltzmann Electron
16:15-16:30	**Loay Khalifa**, *DePaul University (USA)* The Angular Fractal Dimension as a Measure of the Inhomogeneity in the Galaxy Clusters Distribution in the Redshift Range (Z=0-1)
16:30-16:45	**Satoshi Tanaka**, *University of Tsukuba (Japan)* Higher-order Vlasov-Poisson Simulation for Large-Scale Simulation with Massive Neutrino
16:45-17:00	**Andrew Wetzel**, *University of California, Davis (USA)* Simulating the Milky Way
17:00-17:15	**Jesus Pulido**, *University of California, Davis; Los Alamos National Laboratory (USA)* Data Reduction Using Lossy Compression for Cosmology and Astrophysics Workflows
17:15-17:30	**Soumi De**, *Syracuse University (USA)* Measurement of the properties of neutron-star and black-hole binaries using PyCBC Inference

Materials 4	
Location: Conference Center, Ballroom B	**Chair:** Michelle Johannes
16:00-16:15	**Michael Mehl**, *United States Naval Academy (USA)* Learning About Crystallography By Designing a Web Page
16:15-16:30	**Timur Bazhirov**, *Exabyte Inc (USA)* Enabling accessible high-fidelity high-throughput computational design of electronic materials from first principles.
16:30-16:45	**Andrew Morris**, *University of Birmingham (United Kingdom)* *Ab initio* prediction of the structure of Extreme Nanowires Encapsulated within Cabon Nantoubes.
16:45-17:00	**Rossitza Pentcheva**, *University of Duisburg-Essen (Germany)* Confinement-driven electronic and topological phases in corundum-derived oxide honeycomb superlattices
17:00-17:15	**David Quigley**, *University of Warwick (United Kingdom)* Computational study of functional properties in extreme nanowires
17:15-17:30	**Shunda Chen**, *University of California, Davis (USA)* Effects of chemical intercalation, strain and phase transition on heat transport in bulk and single-layer MoS_2: First-principles calculations
17:30-17:45	**Hisazumi Akai**, *University of Tokyo (Japan)* Calculated Seebeck coefficient of transition-metal elements Calculated Seebeck coefficient of transition-metal elements
17:45-18:00	**Florian Libisch**, *TU Wien (Austria)* Edge-free graphene quantum dots on hexagonal boron nitride

Software 2	
Location: Conference Center, Ballroom C	**Chair:** Jeremy Mason
16:00-16:15	**Andrew Horsfield**, *Imperial College London (United Kingdom)* Gaussian Tight Binding: like DFT, but much faster
16:15-16:30	**Jun Zhou**, *National University of Singapore (Singapore)* Two dimensional materials design by high-throughput calculations
16:30-16:45	**Noriko Akutsu**, *Osaka Electro-Communication University (Japan)* Driving force dependence of the height of a faceted macrostep in non-equilibrium steady-state crystal growth
16:45-17:00	**Arnulf Möbius**, *IFW Dresden (Germany)* Simulated annealing, effective but inefficient? A case study for the 3D136 instance of the HP model of protein folding
17:00-17:15	**Alfred Farris**, *University of Georgia, Athens (USA)* An Improved Multicanonical Monte Carlo Algorithm for the Basis Expansion of the Density of States
17:15-17:30	**Johannes Voss**, *SLAC National Accelerator Laboratory (USA)* Efficient reduced density matrix functional theory with model interactions for solids
17:30-17:45	**Cale Harnish**, *University of Notre Dame (USA)* An Adaptive Wavelet Algorithm for Multi-Resolution Modeling in *n*-Dimensions with Error Control

Wednesday, August 1

	Plenary Session *Location: Conference Center, Ballroom ABC* *Chair: Richard Scalettar*
09:00-09:45	**Noa Marom**, *Carnegie Mellon University (USA)* *Recipient of the 2018 IUPAP Young Scientist Prize in Computational Physics* Molecular Crystal Structure Prediction with GAtor and Genarris
09:45-10:30	**Emanuel Gull**, *University of Michigan (USA)* Diagrammatic and Continuous Time Quantum Monte Carlo
10:30-11:00	**Break**
	Plenary Session *Location: Conference Center, Ballroom ABC* *Chair: Richard Scalettar*
11:00-11:45	**Silke Biermann**, *CPHT, Ecole Polytechnique (France)* First principles calculations for materials with strong electronic Coulomb correlations – where do we stand?
11:45-12:30	**Philip Hopkins**, *California Institute of Technology (USA)* Developments in Quasi-Lagrangian Moving-Mesh and Mesh-Free Methods: Applications to Fluid Dynamics, Cosmology, Plasmas, Collisionless and Elastic Dynamics
12:30-14:00	**Lunch** *(Buehler Alumni Center)*
14:00-15:30	**Parallel Sessions 1** **Materials 5**, *Conference Center, Ballroom A* **Materials 6**, *Conference Center, Ballroom B* **Algorithms 1**, *Conference Center, Ballroom C*
15:30-16:00	**Break**
16:00-18:00	**Parallel Sessions 2** **Software 3**, *Conference Center, Ballroom A* **Materials 7**, *Conference Center, Ballroom B* **Algorithms 2**, *Conference Center, Ballroom C*
18:00-21:00	**Banquet** *Location: Buehler Alumni Center* ***Banquet Speaker*** **Tony DeRose**, *PIXAR Animation Studios* Computational Physics at Pixar

Wednesday, Parallel Sessions 1

Materials 5	
Location: Conference Center, Ballroom A	**Chair:** Antia Botana
14:00-14:45	**Invited: Michelle Johannes**, *Naval Research Laboratory (USA)* How Materials Physics Drives Li-ion Battery Performance
14:45-15:30	**Invited: Jack Wells**, *Oak Ridge National Laboratory (USA)* Enabling Large-Scale Physics Applications on Summit Through the Center for Accelerated Application Readiness

Materials 6	
Location: Conference Center, Ballroom B	**Chair:** Rossitza Pentcheva
14:00-14:45	**Invited: Renata Wentzcovitch**, *Columbia University (USA)* Spin Crossover in Lower Mantle Minerals
14:45-15:30	**Invited: Vasily Bulatov**, *Lawrence Livermore National Laboratory (USA)* Predictive simulations of crystal plasticity: multiscale or cross-scale?

Algorithms 1	
Location: Conference Center, Ballroom C	**Chair:** Ehsan Khatemi
14:00-14:45	**Invited: Helmut G. Katzgraber**, *Texas A&M University (USA); 1QB Information Technologies (Canada)* Quantum-driven classical optimization
14:45-15:30	**Invited: Sergio Boixo**, *Google (USA)* The Question of Quantum Supremacy

Wednesday, Parallel Sessions 2

Software 3	
Location: Conference Center, Ballroom A	**Chair:** Antia Botana
16:00-16:15	**Denis Jarema**, *Max Planck Institute for Plasma Physics (Germany)* Minimally Invasive Adaptation of Computational Grids for Gyrokinetic Eulerian Simulations
16:15-16:30	**Constancio Miguel Arizmendi**, *Universidad Nacional de Mar del Plata (Argentina)* Heat Transport on Brownian Motors
16:30-16:45	**David Landau**, *University of Georgia, Athens (USA)* A First Look at Lattice Effects in Coarse-Grained Protein Models via Wang-Landau Simulations
16:45-17:00	**Masako Takasu**, *Tokyo University of Pharmacy and Life Sciences (Japan)* Analysis of Inhomogeneity: Brownian Dynamics Simulations of Tetra-Peg Gel Formation
17:00-17:15	**Atul Kumar Verma**, *IIT Ropar (India)* Modelling of stochastic transport problems using exclusion processes
17:15-17:30	**Zhijun Shen**, *Institute of Applied Physics and Computational Mathematics (China)* Overcoming the Carbuncle Instability for the HLLC-type Riemann Solver
17:30-17:45	**Umar Bala**, *Federal Polytechnic, Bauchi (Nigeria)* Viscoelastic Flow With Partial Slip Through a Two Heated Plate Influenced by Magnetic Field

Materials 7	
Location: Conference Center, Ballroom B	**Chair:** Rossitza Pentcheva
16:00-16:15	**Jeremy Mason**, *University of California, Davis (USA)* Classification of Atomic Environments using the Gromov-Wasserstein Distance
16:15-16:30	**Elad Segev**, *Ben-Gurion University of the Negev (Israel)* Discovering a Novel Nanometric Cubic Phase in Monochalcogenide Semiconductors – The Critical Role of Adsorbed Ligands
16:30-16:45	**Mit H. Naik**, *Indian Institute of Science (India)* Ultraflat bands and shear solitons in Moiré patterns of twisted bilayer transition metal dichalcogenides.
16:45-17:00	**Regina Maphanga**, *Council for Scientific and Industrial Research, Pretoria (South Africa)* Density Functional Theory Studies of Graphene/Sodium Oxide Composites
17:00-17:15	**Huilong Yu**, *China Academy of Engineering Physics, Jiangyou (China)* Microscopic behavior of hydrogen on PuO_2(110) surfaces from first principles calculations
17:15-17:30	**Merve Baksi**, *Middle East Technical University (Turkey)* Ab Initio Investigation of Nanotribological Properties of the Hexagonal BN/Au(111) Interface
17:30-17:45	**Mitsuyoshi Tomiya**, *Seikei University (Japan)* I-V Characteristics of In-Plate Graphene Nanoribbon/h-BN Heterojunctions and Resonant Tunneling

Algorithms 2	
Location: Conference Center, Ballroom C	**Chair:** Ehsan Khatemi
16:00-16:15	**Tasrief Surungan**, *Hasanuddin University (Indonesia)* Phase diagram of six-state clock model on rewired square lattices
16:15-16:30	**Urs R. Hähner**, *ETH Zurich (Switzerland)* DCA++ project: Sustainable and scalable development of a high-performance research code
16:30-16:45	**Matthew Jones**, *Colorado School of Mines; Nvidia Corporation (USA)* QuSP: The Quantum Simulator Package
16:45-17:00	**Li Haipeng**, *China University of Mining and Technology (China)* Alkyl group functionalization–induced thermal conductivity attenuation in graphene nanoribbons
17:00-17:15	**Artur Tamm**, *Lawrence Livermore National Laboratory (USA)* Electronic Stopping as a Function of Local DensityElectronic Stopping as a Function of Local Density
17:15-17:30	**Cheng-Wei Lee**, *University of Illinois, Urbana-Champaign (USA)* Charge equilibration and electronic stopping for silicon projectiles in silicon

Thursday, August 2

	Plenary Session *Location: Conference Center, Ballroom ABC* *Chair: Ching Fong*
09:00-09:45	**Michael Biercuk**, *University of Sydney (Australia)* Building quantum control solutions using filter functions as an efficient computational tool
09:45-10:30	**Chris Wolverton**, *Northwestern University (USA)* Using Artificial Intelligence to Discover New Materials
10:30-11:00	**Break**
	Plenary Session *Location: Conference Center, Ballroom ABC* *Chair: Ching Fong*
11:00-11:45	**Julia Yeomans**, *University of Oxford (United Kingdom)* Self-propelled topological defects in active matter
11:45-12:30	**Ribhu Kaul**, *University of Kentucky (USA)* Zero temperature phase diagrams of two dimensional quantum spin models
12:30-14:00	**Lunch** *(Buehler Alumni Center)*
14:00-15:30	**Parallel Sessions 1** **Soft Matter 1**, *Conference Center, Ballroom A* **Materials 8**, *Conference Center, Ballroom B* **Quantum Many-body 3**, *Conference Center, Ballroom C*
15:30-16:00	**Break**
16:00-18:00	**Parallel Sessions 2** **Soft Matter 2**, *Conference Center, Ballroom A* **Materials 9**, *Conference Center, Ballroom B* **Quantum Many-body 4**, *Conference Center, Ballroom C*

Thursday, Parallel Sessions 1

Soft Matter 1	
Location: Conference Center, Ballroom A	**Chair:** Soham Ghosh
14:00-14:45	**Invited: Yuko Okamoto**, *Nagoya University (Japan)* Enhanced sampling methods for spin systems and biomolecular systems
14:45-15:00	**Lianghui Gao Gao**, *Beijing Normal University (China)* Mechanisms of Antimicrobial Peptide-Induced Vesicle Shape Transformation and Pore Formation
15:00-15:15	**Barbara Jones**, *IBM Research - Almaden (USA)* Dynamics of Viral Mutation and Evolution
15:15-15:30	**Sunita Negi**, *Amity University, Gurgaon, India* Effect of varying environmental conditions on the conformation change of a protein

Materials 8	
Location: Conference Center, Ballroom B	**Chair:** Michael Mehl
14:00-14:45	**Invited: Koblar Jackson**, *Central Michigan University (USA)* Fermi-Löwdin orbital self-interaction correction: efficient density functional theory calculations without self-interaction
14:45-15:00	**Elmar Bittner**, *ITP, Heidelberg University (Germany)* On the interface tension of the Ising model
15:00-15:15	**Martin Weigel**, *Coventry University (Germany)* Adaptive population Monte Carlo simulations
15:15-15:30	**Hendrik Schawe**, *Universität Oldenburg (Germany)* Large Deviations of Convex Hulls of Self-Avoiding Random Walks

Quantum Many-body 3	
Location: Conference Center, Ballroom C	**Chair:** Giacomo Resta
14:00-14:45	**Invited: Zi Yang Meng**, *Institute of Physics, Chinese Academy of Sciences (China)* Quantum Monte Carlo investigations of correlated electron systems, present and future
14:45-15:00	**Ying Wai Li**, *Oak Ridge National Laboratory (USA)* A computational framework for model Hamiltonian construction from materials properties
15:00-15:15	**Brian Moritz**, *SLAC National Accelerator Laboratory; Stanford University (USA)* Fluctuating stripes in Hubbard models of high-T_c cuprate superconductors
15:15-15:30	**Rossitza Pentcheva**, *University of Duisburg-Essen (Germany)* Time-evolution of optical excitations in Fe/MgO(001) superlattice from RT-TDDFT

Thursday, Parallel Sessions 2

Soft Matter 2	
Location: Conference Center, Ballroom A	**Chair:** Soham Ghosh
16:00-16:15	**Zewen Zhang**, *University of Georgia, Athens (USA)* Thermodynamic and Structural Similarity of Crambin Lattice Protein Homologues
16:15-16:30	**Matthew Kroonblawd**, *Lawrence Livermore National Laboratory (USA)* Predicted pathways for chemical degradation in siloxane polymers following phenyl excitations
16:30-16:45	**Richard Kriske** It May be Possible to construct a “Reversible” Computer out of Capillary Tubes
16:45-17:00	**Doniyor Babajanov**, *Turin Polytechnic University in Tashkent (Uzbekistan)* Charge transport in branched conducting polymers: Quantum graphs based approach
17:00-17:15	**José Ruiz-Franco**, *Sapienza-Università di Roma (Italy)* Equilibrium colloidal gels under shear

Materials 9	
Location: Conference Center, Ballroom B	**Chair:** Michael Mehl
16:00-16:15	**Lev Shchur**, *Science Center in Chernogolovka (Russia)* Fractal dimension of percolating interface in the spatial evolutionary games
16:15-16:30	**Xia Cui**, *IAPCM Beijing (China)* Asymptotic-Preserving Simulation Methods for Non-Equilibrium Radiation Diffusion Problem
16:30-16:45	**Warren E. Pickett**, *University of California, Davis (USA)* Hole Doping of the Weak Itinerant Antiferromagnet TiAu
16:45-17:00	**Adlane Sayede**, *Université d'Artois (France)* New insight for hydrogen storage in the magnesium nickel and magnesium copper systems
17:00-17:15	**Vipin Kumar**, *Sardar Vallabhbhai National Institute of Technology (India)* Structure, Electronic, Vibrational Properties of Stanane and its Application as a Potential Gas Sensor
17:15-17:30	**Chaib Youness**, *University of Casablanca (Morocco)* First principles study electronic properties of (110) surface GaAs/GaN nanowires
17:30-17:45	**Sitangshu Bikas Santra**, *Indian Institute of Technology Guwahati (India)* Discontinuous transition in a random growth lattice filling model of percolation

Quantum Many-body 4	
Location: Conference Center, Ballroom C	**Chair:** Giacomo Resta
16:00-16:15	**Xiao Zhang**, *University of Illinois, Urbana-Champaign (USA)* Near-edge Absorption of HfO_2: Effect of Excitons
16:15-16:30	**Li Huang**, *China Academy of Engineering Physics, Mianyang (China)* Combining many-body perturbation theory with dynamical mean-field theory
16:30-16:45	**Isha Dhiman**, *Thapar Institute of Engineering and Technology (India)* The role of coupling constant in an inhomogeneous two-lane exclusion process model
16:45-17:00	**Sarun Phibanchon**, *Burapha University (Thailand)* Two-dimensional solitary wave solution to the quadratic-cubic nonlinear Schrodinger equation
17:00-17:15	**Songvudhi Chimchinda**, *Burapha University (Thailand)* Adomian Decomposition Method for the dark solitons solution to the modified Korteweg-de Vries equation
17:15-17:30	**Yuan Ping**, *University of California, Santa Cruz (USA)* Charged Defects in Two-dimensional Materials from Many Body Perturbation Theory

Poster Session

Tuesday, July 31 from 18:00-21:00

Conference Center

1 Algorithm Development	
1.1	**Chuang Chen**, *Institute of Physics, Chinese Academy of Sciences (China)* Symmetry Enforced Self-Learning Monte Carlo Method Applied to the Holstein Model
1.2	**Krishnakumar Bhattaram**, *San Jose State University (USA)* Boosting convergence of numerical linked-cluster expansions with the Lanczos algorithm
	Vasily Buyadzhi, *Odessa State Environmental University (Ukraine)* DAMAGE ANALYSIS AND DETECTION UNDER VARYING ENVIRONMENTAL AND OPERATIONAL CONDITIONS USING A CHAOS THEORY METHODS: ADVANCED COMPUTATIONAL CODE
	Valentin Ternovsky, *Odessa State Environmental University (Ukraine)* ADVANCED COMPUTATIONAL APPROACH TO STUDYING RYDBERG AND AUTOIONIZATION SPECTRA OF HEAVY ATOMS
	Brian Ferrari, *University of Central Florida, Orlando (USA)* A Comparison of Medium-Sized Basis Sets for the Prediction of Geometries, Vibrational Frequencies, Infrared Intensities and Raman Activities

2 Astrophysics	
2.1	**Sijo Sebastian**, *St. Berchman's College (India)* Effects of Pressure Anisotropy on Solitary Waves in Multi-ion Plasmas
2.2	**Rohit Sharma**, *Satyam Institute of Engineering & Technology (India)* Study of Thermodynamic Properties of Hydrogen Thermal Plasma in Local Thermodynamic Equilibrium Including Pressure Derivative of Partition Function
	Cameron Woo, *Independent, Independent (USA)* X-Ray Source Distribution and the Discovery of 14 New Black Hole Candidates within the Milky Way
	Dong Hoon Lee, *St. Andrew's School (USA)* NuSTAR Search for Black Holes within the Galactic Center
	Shankar Bhattarai, *Tribhuvan University (Nepal)* Space Debris Removal Mechanism Using CubeSat with Gun Shot Facilities
	Vasily Buyadzhi, *Odessa State Environmental University (Ukraine)* MULTI-PHOTON SPECTROSCOPY OF THE DEBYE PLASMAS ATOMIC SYSTEMS IN A ONE- AND TWO-COLOR LASER FIELDS: ADVANCED COMPUTATIONAL APPROACH

3 Computational Physics Education	
	Raji Heyrovska, *Academy of Sciences of the Czech Republic (Czech Republic)* Modification of Bohr's equation for the energy of hydrogen atom

4 Energy, Environment and Climate Modeling	
4.1	**Fernanda Bononi**, *University of California, Davis (USA)* Modeling the Absorption Spectra of Organic Molecules at the Ice-Air Interface
	Alexander Glushkov, *Odessa State Environmental University (Ukraine)* NEW COMPUTATIONAL APPROACH TO THE EARTH ATMOSPHERE LARGE-SCALE PROCESSES AND ANGLE MOMENTUM BALANCE MODELLING: ATMOSPHERIC CIRCULATION, TELECONNECTION AND RADIO-WAVEGUIDES
	Alexander Glushkov, *Odessa State Environmental University (Ukraine)* AN ADVANCED CHAOS-GEPMETRIC COMPUTATIONAL APPROACH TO ANALYSIS, PROCESSING, PREDICTION OF ENVIRONMENTAL MEASUREMENTS DATA: AIR POLLUTION

5 Fluid Dynamics	
	Olga Khetselius, *Odessa State Environmental University (Ukraine)* NEW COMPUTATIONAL APPROACH TO MODELLING DYNAMICS OF ATMOSPHERE VENTILATION AND INDUSTRIAL CITY'S AIR POLLUTION ANALYSIS

6 Lattice Field Theory in Particle and Nuclear Physics	
	Valentin Ternovsky, *Odessa State Environmental University (Ukraine)* NEW COMPUTATIONAL APPROACH TO HADRONIC ATOMIC SYSTEMS: RADIATIVE AND STRONG INTERACTION CORRECTIONS

7 Materials Physics	
7.1	**Hongyu Yu**, *Jilin University (China)* Molecular dynamic study of solid-state transitions of ammonium nitrate
7.2	**Chung-Yuan Ren**, *National Koahsiung Normal University (Taiwan)* Application of Van Der Waals Density Functionals to Two Dimensional Systems Based on a Mixed Basis Approach
7.3	**Defang Duan**, *Jilin University (China); University of Cambridge (United Kingdom)* Novel superconductivity in ternary hydrides $MAlH_6$ (M= Li, Mg) under high pressure
7.4	**Giuseppe Barbalinardo**, *University of California, Davis (USA)* UNRAVELING A NEW HEAT TRANSPORT REGIME AT THE NANOSCALE
7.5	**Sul-Ah Ahn**, *Korea Institute of Science and Technology Information (Republic of Korea)* A Detailed Numerical Analysis for High-T_c Superconductivity Phase Diagram Based on U(1) Slave-Boson Approach to the *t-J* Hamiltonian
7.6	**Chunjing Jia**, *SLAC National Laboratory (USA)* Numerical simulation of resonant inelastic x-ray scattering: a Wannier-orbital based method
	Doniyor Babajanov, *Turin Polytechnic University in Tashkent (Uzbekistan)* Quantum transport in driven networks of harmonic oscillators
	Da Li, *JiLin University (China)* Pressure-Induced Superconducting Ternary Hydride H_3SXe: A Theoretical Investigation
	SRUTHI T, *National Institute of Technology (India)* Enhancement of Quantum Capacitance by Chemical Modification of Graphene and ZigzagGraphene Nano-ribbon Supercapacitor Electrodes: A First PrinciepleCalculation.
	Emmanuel Igumbor, *University of Pretoria (South Africa)* Defect levels induced by double substitution of B and N in 4H-SiC: a hybrid density functional study
	Prabhat Ranjan, *Manipal University Jaipur (India)* Computational Analysis of Au_nV(n=1-8) Nanoalloy Clusters Invoking Density Functional Theory Based Descriptors

7 Materials Physics (continue)	
	Abdiravuf Dzhurakhalov, *University of Antwerp (Belgium)* Computer simulation of the interaction of fullerene with carbon clusters C_n (n=3-6)
	Ibarhim Buba Garba, *Federal University Gashua (Nigeria)* Ab Initio Investigation of Electronic Properties and Lattice Thermal Conductivity of Zincblende Indium Nitride (InN)
	Mahdieh Aghajani, *Sharif University of Technology (Iran)* Chemical and Mechanical pressure dependence of structural, magnetic and electronic properties of $BaFe_2As_2$: Density functional study
	Asif Iqbal Bhatti, *Institut polytechnique de Grenoble (France)* First principles investigation of transition-metal complexes for battery application
	C Morante, *San Jose State University (USA)* External field dependences of local magnetic fields in single crystals of Fe_3O_4: a Maximum-Entropy μSR study.
	Vladimir Fedorov, *Moscow Institution of Physics and Technology (Russia)* Thermodynamic model of the laser beam distribution analysis system based on matrix of piezoelectric crystals
	Miqdad Raza, *University of California, Davis (USA)* Sodium Ion Conduction in Germanium Phosphide and Germanium Arsenide
	Thanh Cuong Nguyen, *University of Tsukuba (Japan)* *In silico* synthesis of monolayer B_3N_3-doped graphene with high thermoelectric power
	Charles Sievers, *University of California, Davis (USA)* Thermal Transport Across Graphene Step Junctions

8 Novel Hardware and Software Paradigms	
8.1	**Dustin Sanford**, *CASPER (USA)* Self-Consistent Simulation of Dust-Plasma Interactions in a Complex Plasma

9 Quantum Many-Body Physics	
9.1	**Priyadarshini Kapri**, *Indian Institute of Technology Guwahati (India)* Tunable refrigeration properties of Rashba coupled nano-junction devices
9.2	**Sunayana Dutta**, *Indian Institute of Technology Guwahati (India)* Tunneling Dynamics of interacting bosons in a quantum seesaw potential
9.3	**Bowen Zhao**, *Boston University (USA)* Symmetry enhanced first-order phase transition in a two-dimensional quantum magnet
9.4	**Boris Daniel Gutiérrez Cortés**, *University of the Pacific, Stockton (USA)* Translationally transformed coupled-cluster theory in a local basis for periodic systems
9.5	**Kristopher McBrian**, *San Jose State University (USA)* Learning Thermodynamics of the Transverse Field Ising Model
9.6	**Stephan Humeniuk**, *Institute of Physics, Chinese Academy of Sciences, Beijing (China)* Full counting statistics in the two-dimensional Hubbard model
	Olga Khetselius, *Odessa State Environmental University (Ukraine)* ADVANCED COMPUTATIONAL APPROACH IN LASER ELECTRON-GAMMA-NUCLEAR SPECTROSCOPY OF ATOMS: “SHAKE-UP” AND NEET EFFECTS
	Olga Khetselius, *Odessa State Environmental University (Ukraine)* COMPUTING HYPERFINE STRUCTURE OF HEAVY ATOMS AND MULTICHARGED IONS WITHIN OPTIMIZED RELATIVISTIC MANY-BODY PERTURBATION THEORY
	Alexander Glushkov, *Odessa State Environmental University (Ukraine)* ADVANCED COMPUTATIONAL APPROACH TO HEAVY ATOMS AND NUCLEI IN A STRONG LASER FIELD:DC, AC STARK EFFECT, MULTIPHOTON RESONANCES
	Vasily Buyadzhi, *Odessa State Environmental University (Ukraine)* AN ADVANCED RELATIVISTIC ENERGY APPROACH IN ELECTRON-COLLISIONAL SPECTROSCOPY OF MULTICHARGED IONS IN PLASMAS
	Andrey Svinarenko, *Odessa State Environmental University (Ukraine)* ADVANCED COMPUTATIONAL APPROACH TO RYDBERG ATOMS IN A BLACK-BODY RADIATION FIELD

9 Quantum Many-Body Physics (continue)	
	Eugeny Ternovsky, *Odessa State Environmental University (Ukraine)* COMPUTING RADIATIVE SPECTRAL PARAMETERS OF MULTICHARGED IONS WITHIN RELATIVISTIC ENERGY APPROACH AND MODEL POTENTIAL METHOD
	Eugeny Ternovsky, *Odessa State Environmental University (Ukraine)* RELATIVISTIC COMPUTING EXCITED AND AUTOIONIZING STATES SPECTROSCOPIC PARAMETERS FOR SOME MULTICHARGED IONS
	Deng-Ruei Tan, *National Taiwan Normal University, Taipei (Taiwan)* Universal quantum critical at finite temperature for two-dimensional disordered and clean dimerized spin-1/2 anitferromagents

10 Soft matter and Biological Physics	
10.1	**Hwankyu Lee**, *Dankook University (Republic of Korea)* Molecular modeling of polymer-grafted carbon nanotubes interacting with lipid membranes
10.2	**Hibiki Itoga**, *Tokyo University of Pharmacy and Life Sciences (Japan)* Monte Carlo simulation of transformation of vesicle induced by internal particles
10.3	**Takao Otsuka**, *RIKEN (Japan)* Quantum chemical analysis of reaction indices and reaction path for drug molecules
10.4	**Hiroaki Saito**, *RIKEN (Japan)* Molecular dynamics study on the free energy profiles of lipid translocation across binary POPC bilayer mixtures
10.5	**Taku Mizukami**, *JAIST (Japan)* Molecular dynamic study on solvation free energy of water and model protein

11 Statistical Mechanics and Complex Systems	
11.1	**Przemyslaw Gawronski**, *AGH University of Science and Technology (Poland)* The coevolving voter model with spin-dependent probability of rewiring
11.2	**Jun Takahashi**, *Institute of Physics, Chinese Academy of Sciences, Beijing (China)* Studying emergent symmetry at a first-order transition with a simple model
	Abiodun Egunjobi, *Moshood Abiola Polytechnic; Federal University of Agriculture (Nigeria)* Synchronization in Nonlinear Oscillators Using A SingleVariable Control: Theory and Experiment.
	E Ghorbani, *San Jose State University (USA)* 2-Dimensional Frustration Modeling
	Akbari Jahan, *NERIST, Nirjuli (India)* Evaluation of Bose-Einstein integral functions
	Valentin Ternovsky, *Odessa State Environmental University (Ukraine)* ADVANCED COMPUTATIONAL APPROACH TO NONLINEAR DYNAMICS OF LASER SYSTEMS WITH ELEMENTS OF A CHAOS
	Andrey Svinarenko, *Odessa State Environmental University (Ukraine)* ADVANCED COMPUTATIONAL APPROACH TO DIATOMIC MOLECULES IN AN ELECTROMAGNETIC FIELD: MOLECULAR POLARIZABILITIES AND CHAOS