CCQ

International Workshop on Recent Developments in Electronic Structure (ES21)

Workshop
Monday July 12th – Thursday July 15th, 2021 11:00 a.m. – 6:00 p.m. Eastern Daylight Time(EDT)
Center for Computational Quantum Physics
Virtual

For over 30 years, the Annual Workshop on Recent Developments in Electronic Structure Methods has brought together participants in electronic structure theory from universities, colleges, institutes and laboratories around the world.

To continue the tradition of this workshop series, the Center for Computational Quantum Physics (CCQ) at the Flatiron Institute is pleased to virtually host ES21. In addition to invited talks, the workshop will include poster

presentations and small group discussion sessions. We hope this will provide an occasion for the community to gather after a very challenging year, hear about the latest developments, and discuss the future of electronic structure methods.

Registration is now closed The workshop is free but registration is required. On the registration form, you will be asked to indicate if you would like to present a poster (submission deadline for poster title is June 21st) and to indicate your preferred topics for the small group discussions.

Local Organizers

- Shiwei Zhang
- Tim Berkelbach
- Cyrus Dreyer

International Steering Committee

- Susan Atlas (U. New Mexico)
- Jerry Bernholc (NC State)
- Marco Buongiorno Nardelli (Univ. North Texas)
- Roberto Car (Princeton)
- David Ceperley (UIUC)
- James Chelikowsky (UT Austin)
- Mei-Yin Chou (Academia Sinica, Taiwan)
- Natalie Holzwarth (Wake Forest)
- Steven G. Louie (UC Berkeley)
- Richard M. Martin (UIUC, Stanford)
- Normand A. Modine (Sandia)
- Andrew Rappe (UPenn)
- John J. Rehr (Washington)
- David Strubbe (UC Merced)
- Cyrus Umrigar (Cornell)
- David Vanderbilt (Rutgers)
- Lucas K. Wagner (UIUC)
- Shiwei Zhang (Flatiron)

Special Guest Speakers

David Spergel	Simons Foundation
Richard Martin	University of Illinois and Stanford

Confirmed Invited Speakers

Yang-Hao Chan	IAMS, Academia Sinica, Taiwan
Martin Claassen	University of Pennsylvania
Valentino Cooper	Oak Ridge National Laboratory
Benjamin Fregoso	Kent State University
Liang Fu	Massachusetts Institute of Technology
Antoine Georges	Flatiron Institute, College de France
Stephanie Hansen	Sandia National Laboratory
Heather Kulik	Massachusetts Institute of Technology
Zhenglu Li	University of California, Berkeley and Lawrence Berkeley National Laboratory
Lukas Muechler	Flatiron Institute, Pennsylvania State University
Shyue Ping Ong	University of California, San Diego
Raquel Queiroz	Weizmann Institute of Science
Brenda Rubenstein	Brown University
Sandeep Sharma	University of Colorado, Boulder
James Shee	University of California, Berkeley
Eric L. Shirley	National Institute of Standards and Technology (NIST)

Jagoda Sławińska	University of Groningen
Liang Tan	Molecular Foundry, Lawrence Berkeley National Laboratory
Stepan Tsirkin	University of Zurich
Alexander Wietek	Flatiron Institute

Agenda

Monday, July 12

All times are in Eastern Daylight Time(EDT)

11:00am -11:05am	Shiwei Zhang, Tim Berkelbach, Cyrus Dreyer	*Welcome*	
11:05am - 11:41am (30+6)	James Shee	*A new hope for the quantum-chemical modeling of transition metal compounds*	Abstract
11:41am - 12:17pm (30+6)	Sandeep Sharma	*Mean field and correlated calculations in molecules and solids*	Abstract
12:17pm - 12:53pm (30+6)	Lukas Muechler	*Quantum embedding methods for correlated excited states of point defects: Case studies and challenges*	Abstract
12:53pm - 2:00pm	*Lunch*		
2:00pm - 2:36pm (30+6)	Eric Shirley	*Core holes, core hole memory and space quantization as electronic structure probes*	Abstract
2:36pm - 3:12pm (30+6)	Zhenglu Li	*Linear-response GW perturbation theory (GWPT) method for correlation-enhanced electron-phonon interactions: semiconductors, metals and oxide superconductors*	Abstract
3:12pm - 3:48pm (30+6)	Liang Tan	*Light-induced phase transitions and their effect on photocurrent*	Abstract
3:48pm - 4:00pm	*Break*		

4:00pm - 6:00pm	Poster Session #1		

Tuesday, July 13

11:00am - 11:36am (30+6)	Benjamin Fregoso	*Higher order bulk photovoltaic effects*	Abstract
11:36am - 12:12pm (30+6)	Yang-Hao Chan	*Excitonic effects in optical-field-driven quasi 2D materials from time-dependent GW approach*	Abstract
12:12pm - 12:48pm (30+6)	Stepan Tsirkin	*Towards ab initio theory for nonlinear transport phenomena with Berry-Boltzmann equations and Wannier functions*	Abstract
12:48pm -1:40pm	*Lunch*		
1:40pm - 2:00pm (20)	Richard Martin	*The US Africa Initiative on Electronic Structure and other activities in Africa*	Abstract
2:00pm - 3:00pm	David Spergel	*The role of Simons Foundation in supporting Transformative Science*	
3:00pm - 3:20pm	*Break*		
3:20pm - 5:20pm	Discussion Sessions		

Wednesday, July 14

11:00am - 11:36am (30+6)	Raquel Queiroz	*Origin of topology in the band structure of bismuth*	
11:36am - 12:12pm (30+6)	Liang Fu	*Electronic structure and correlated topological states in semiconductor moire systems*	
12:12pm - 12:48pm (30+6)	Martin Claassen	*Unconventional phases and topology in Moire heterostructures*	
12:48pm - 2:00pm	*Lunch*		
2:00pm - 2:36pm (30+6)	Shyue Ping Ong	*Addressing Errors in Ab Initio Molecular Dynamics Predictions through Machine Learning*	Abstract
2:36pm - 3:12pm (30+6)	Heather Kulik	*(Not quite) doomed to fail: machine learning to detect and overcome limitations of DFT for strongly correlated materials*	Abstract
3:12pm - 3:48pm (30+6)	Jagoda Slawinska	*Modeling of advanced relativistic materials in the PAOFLOW code*	Abstract

3:48pm - 4:00pm	*Break*		
4:00pm - 6:00pm	Poster Session #2		

Thursday, July 15

11:00am - 11:36am (30+6)	Antoine Georges	*Strong Correlations in Multi-Orbital Materials: Beyond Mottness*	Abstract
11:36am - 12:12pm (30+6)	Brenda Rubenstein	*Finite Temperature Auxiliary Field Quantum Monte Carlo in the Canonical Ensemble*	Abstract
12:12pm -12:22pm	*Break*		
12:22pm - 12:58pm (30+6)	Alex Wietek	*Mott insulating states with competing orders in the triangular lattice*	Abstract
12:58pm - 1:34pm (30+6)	Stephanie Hansen	*Benchmarking consistent observable and material properties from an average-atom model to predictions from time-dependent density functional theory*	Abstract
1:34pm - 2:10pm (30+6)	Valentino Cooper	*Computational design strategy for disordered complex oxides*	Abstract
2:10pm - 2:30pm	*Closing*		

Poster Session #1: Monday, July 12, 4-6pm

Lynet Allan	Ab initio study of doping in Titanium based oxides	
Antonios Alvertis	Non-perturbative exciton-phonon interactions in molecular crystals: Impact of exciton delocalization and the effect of molecular size	Poster
Isuru Ariyarathna	Electronic Structure Analysis of Ground and Excited States of HfO	Poster
Oliver Backhouse	Auxiliary second-order Green's function perturbation theory	Poster
Yueqing Chang	Layer-dependent spin-momentum locking in monolayer 1T′-WTe2	Poster
Rene Costa	Zwitterionic or non-ionic conformer structures of betanidin influences to thermodynamic, charge transfer and reactivity indices property towards DSSCs applications.	Poster

Duy-Khoi Dang	Developments in incremental CASSCF	
Brandon Eskridge	Treatment of Spin-Orbit Coupling in Atoms, Molecules, and Solids using Auxiliary-Field Quantum Monte Carlo	Poster
Nicolás Forero	Study of electronic properties in ferroelectric materials with first-principle methods	Poster
Misha Galperin	Auxiliary Master Equation for Nonequilibrium Dual Fermion and Dual Boson Approaches	Poster
Alexandru Georgescu	Machine Learning tools to build databases, identify new features and new materials - application to metal-insulator transition compounds	Poster
Olivier Gingras	Superconducting Symmetries of Strontium Ruthenate	Poster
Gamachis Sakata Gurmesa	Fast 3D-lithium-ion diffusion and high electronic conductivity of Li2MnSiO4 surfaces for rechargeable lithium-ion batteries	Poster
Asnake Haile	Pyridinic Type N-doped Graphene on Cobalt Substrate as Efficient Electrocatalyst for Oxygen Reduction Reaction in Acidic Solution in Fuel Cell	
Natalie Holzwarth	Progress on developing pseudopotential datasets for meta-gga exchange correlation functionals.	Poster
Zhurun Ji	TBD	
Kisung Kang	Phonon, Electron, and Magnon Properties of Antiferromagnetic L10-type MnPt	Poster
Anri Karanovich	Electronic Structure of Mononuclear Cu-based Molecule from Density-Functional Theory with Self-Interaction Correction	Poster
Michelle Kelley	Surface-phonon physics from the semi-dynamical matrix: improved convergence for ab initio prediction of Helium atom scattering (HAS) from 3x1-O/NbO(001)	Poster
Jinwoong Kim	Extracting spin-orbit coupling from a Wannier Hamiltonian	Poster
Destiny Konadu	Mechanism of Guaiacol Hydrodeoxygenation on Cu(111) : Insight from Density Functional Theory	Poster
Edgar Landinez	Gaussian processes for finite size effect extrapolations	Poster
Chenxing Luo	Ab initio investigation of H-bond disordering in δ-AlOOH	Poster
Kevin Ly	Phonons of solid atomic Hydrogen with quantum Monte Carlo	Poster
Md Mehdi Masud	Continuum lowering in compressed silicon	
J. Kevin Nangoi	Ab initio theory of coherent electron-photon-phonon scattering during photoemission: transverse momentum distribution of electrons from PbTe(111) photocathodes as a case study	Poster
Das Pemmaraju	Nonlinear optical response in solids from generalized Kohn-Sham real-time TDDFT	Poster
Yuan Ping	Ab-initio Ultrafast Spin Dynamics in Solids	Poster

Alan Rask	Revealing the Full Spectrum of Electron Correlation in Fe(II)-Porphyrin	Poster
Shang Ren	Quadrupole moments, edge polarizations, and corner charges in the Wannier representation	Poster
Sebastian Reyes-Lillo	Spectroscopic and first principles characterization of electronic, optical and defect properties of p-type CuBi2O4	Poster
Stefan Riemelmoser	RPA-OEP for solids	Poster
Daniel Seleznev	Towards a theory of surface orbital magnetization	Poster
Duo Song	Approach for Enabling High Level Quantum Chemistry in a Periodic Pseudopotential Plane-Wave Basis Set Calculation via Correlation Optimized Virtual Orbitals	Poster
Yang Sun	Iron-rich Fe-O compounds at Earth's core pressures	Poster
Nicodemos Varnava	Axion insulator in a Zintl Compound	
Vyshnavi Vennelakanti	TBD	
Tianqi Wan	Spin state and structural stability of ferropericlase up to 3 Mbar	Poster
Han Wang	Simulating X-ray transient absorption spectroscopy of ultrafast dynamics	Poster
Robert Wexler	Exchange-correlation functional challenges in modeling chalcogenides	Poster
Weronika Wolszczak	Thallium impurity charge states in sodium iodide	

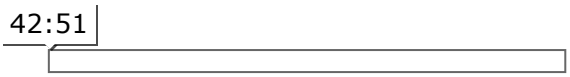
Poster Session #2: Wednesday, July 14, 4-6pm

Tyler Anderson	Nonlocal pseudopotentials and time-step errors in diffusion Monte Carlo	
Xavier Andrade	INQ: a state-of-the-art GPU implementation of DFT and TDDFT	
Timothy Ashani	Thermoelectric Properties, Effective Mass and Fitness function in CuSbS2: Density Functional Theory Approach.	
Diola Bagayoko	Obtaining accurate descriptions of semiconductors with ab-initio density functional theory (DFT) Calculations	Poster
Bradford Barker	The Spin-Flip Bethe Salpeter Equation approach to open-shell electronic structure calculations	Poster

Chanchal Kumar Barman	Broken symmetry driven topological semi-metal to gapped phase transitions in ternary SrAgAs	Poster
John Bonini	Vibro-Polaritons from First Principles	Poster
Brian Busemeyer	Accurate excitations in correlated spin-defects with embedded AFQMC	
Yogesh Chauhan	2d heterostructures	
Siyuan Chen	Electronic density & interatomic forces in solids by plane-wave auxiliary field quantum Monte Carlo	Poster
Rafael Del Grande	Consequences of H Doping in the Electronic and Optical properties of Carbon nanotubes	Poster
Teshome Gerbab Edossa	Study of Electronic and Structural properties of Cadmium Sulfide (CdS) in Zinc-Blend and Wurtizite phase using DFT and DFT+U.	Poster
Jean Baptiste Fankam Fankam	Theoretical investigation of molecular structure, optoelectronic, thermodynamic linear and nonlinear optical properties of 4,5 dibromo-2,7 dinitro-fluorescein	Poster
Arno Förster	Quasiparticle Self-Consistent GW with Vertex Corrections in the Self-Energy	Poster
Alexandru Georgescu	Quantifying the role of the Lattice in Electronic Phase Transitions: Equation of State-Based Formalism and Application to Metal-Insulator Transitions in Ca2RuO3 and RNiO3	Poster
Dipti Jasrasaria	Interplay between surface and interior modes in exciton-phonon coupling at the nanoscale	Poster
Rudranarayan Khatua	Charge Transport and Optoeloectronic Properties of π-conjugated n-type organic materials	
Abhishek Khedkar	Active Space Selection for Multireference Methods	
Minsung Kim	Orbital-selective Mott phase with non-Fermi liquid behavior in FePS3 under pressure	Poster
Kamila Kotur	First-principles study of magnetic bilayer of $NiPS_3$/$FePS_3$	Poster
Adem Külahlioglu	The algebraic diagrammatic construction quantum Monte Carlo method: towards a massively parallel excited state method	
Gionni Marchetti	Assessment of the Approximate Potentials from the RPA Effective Interaction in Condensed Matter Systems	Poster
Verena Neufeld	Ab initio structure of metals from coupled-cluster theory with optimized Gaussian basis sets	Poster
Christian Njeumen	Computational studies of reactivity descriptors, electronic and nonlinear optical properties of multifunctionalized fullerene ylide with acetylsalicylic acid	
Falonne Bertholde Sharone NKOU	Theoretical Insights Into Magnetization In Graphene Containing Single And Interacting Nanoporous Defects	Poster

Akinola Olayinka	Temperature-dependent Thermoelectric Prediction using Machine Learning	
Chin Shen Ong	In-Situ Pseudopotentials for Electronic Structure Theory	Poster
Ezekiel Oyeniyi	Efficient calculation of excitation energies and absorption spectra of nanoclusters	Poster
Jayachandran Peethambaran	Polycrystals as better magnetoelectrics	Poster
Babu Baijnath Prasad	Tunable spin Hall and spin Nernst effects in Dirac nodal line semimetals XCuYAs (X=Zr, Hf; Y=Si, Ge)	Poster
Benjamin Rudshteyn	Benchmark Quantum Chemical Calculations for Transition Metal Complexes via Auxiliary Field Quantum Monte Carlo	Poster
Mihir Ranjan Sahoo	Magnetic phase transition of Mn dimer on graphene doped h-BN through external electric field	Poster
Gautam Sharma	The effect of electron phonon interactions on transport properties of ZrS2 monolayer	Poster
Manas Sharma	Modeling nonlinear optical response of functionalized surfaces	Poster
Puja Singhvi	Electronic and Optoelectronic Properties of Surface-Mounted Metal-Organic Frameworks	Poster
Dmitry Skachkov	First-Principles Method for Schottky Barrier	Poster
Xiao Wang	Ab initio optical absorption spectra for solids with periodic coupled-cluster theory	
Daniel Wines	A first-principles Quantum Monte Carlo study of two-dimensional (2D) GaSe and GaSSe alloys	Poster
Tomasz Woźniak	Exciton g-factors of van der Waals structures from first principles	Poster
Yi Yao	Progress and Outlook Regarding Eigenvalue and Density Matrix Solutions Across Platforms via the ELSI Interface	Poster
Nusaiba Zaman	Study of Small Bimetallic Clusters Agn-1M (M = Au, Co, Cu, Ni, Pd, Pt; n = 3, 9, 15) using Density Functional Theory	
Ruiyi Zhou	Dynamical transition orbitals: A particle–hole description in real-time TDDFT dynamics	Poster

Videos Day 1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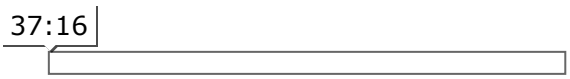
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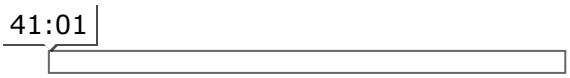
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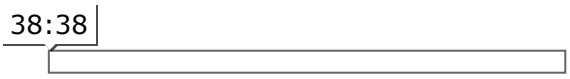
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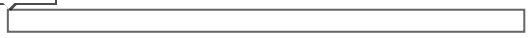

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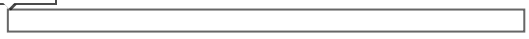

Videos Day 2

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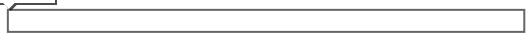

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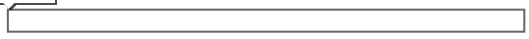

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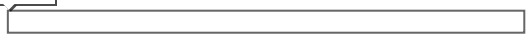

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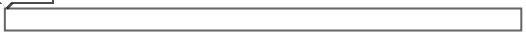

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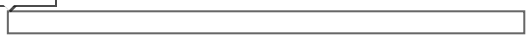

Videos Day 3

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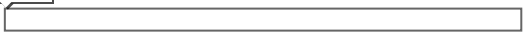

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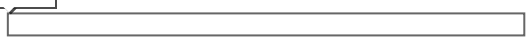

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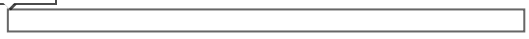

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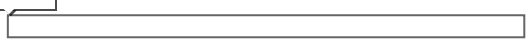

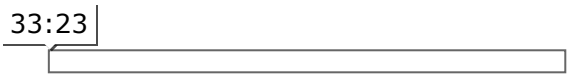
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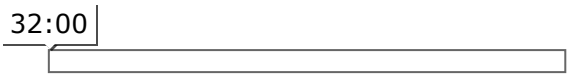
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Videos Day 4

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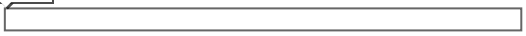

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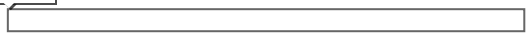

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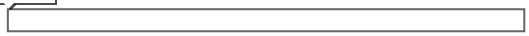

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