TDDFT and Excited States School and Workshop at Rutgers Newark: Workshop Schedule, July 5—8, 2023

Wednesday July 5

8.00am—8.40am Breakfast

8.40—8.45am: Opening Remarks

8.45—9.15am: **Carsten Ullrich**, University of Missouri
TDDFT for excitons in solids

9.15am – 9.45am: **Stefan Kurth,** Ikerbasque UPV/EHU
Mott Metal-Insulator Transition from Steady-State Density Functional Theory

9.45 – 10.15am: **Stefano Pittalis**, National Research Council, Modena, Italy
Progress in ensemble density functional theory for excited states

10.15 – 10.45am: TDDFTea and Coffee

10.45 – 11.15am: **Alberto Castro,** University of Zaragoza, Spain
Floquet engineering quantum systems with optimal control theory

11.15 – 11.45pm: **Hardy Gross,** Hebrew University of Jerusalem
Ultra-fast processes and the challenge of decoherence and thermalization

11.45—2:00pm: Lunch

2.00 – 2.30pm: **Kalman Varga,** Vanderbilt University
TDDFT approach to describe the interaction of matter and light

2.30 – 3.00pm: **Andrew Baczewski,** Sandia National Lab
Improving high-energy-density diagnostics with real-time TDDFT

3.00 – 3.30pm: **Yasuke Kanai,** University of North Carolina
Periodic RT-NEO-TDDFT for Coupled Quantum Dynamics of Electrons and Protons in Heterogeneous System

3.30 – 4.00pm: TDDFTea and Coffee

4.00 – 4.30pm: **Andre Schleife,** University of Illinois, *Electron relaxation and hot-electron-mediated diffusion within real-time TDDFT*

4.30 – 5.00pm: **Christine Aikens,** Kansas State University
TDDFT+TB Gradients and RT-TDDFT Studies of Electron Dynamics

Thursday July 6

8.00am—8.40am Breakfast

8.45 – 9.15am: **Adam Wasserman,** Purdue University
Stretching Bonds Without Breaking Symmetries

9.15 – 9.45am: **Raphael Ribeiro**, Emory University
Spectral statistics and localization of excited-states in optical resonators

9.45 – 10.15am: **Shane Parker,** Case Western University
TDDFT-ris: A minimal auxiliary basis method for low-cost spectra and accelerating ab initio calculations

10.15 – 10.45am: TDDFTea and Coffee

10.45 – 11.15am: **Zhenfei Liu,** Wayne State University
Towards accurate electronic structure calculations of heterogeneous interfaces

11.15 – 11.45am: **Kieron Burke,** University of California Irvine
Which is better, TDDFT or ensemble DFT? Or are they both Gross?

11.45—2pm: Lunch

2.00 – 2.30pm: **Christine Isborn,** University of California Merced*: Using machine learning to establish the importance of high-level electronic structure*

2.30 – 3.00pm: **Daniel Nascimento,** University of Memphis
Exploring perturbative approaches for the simulation of core-level spectra within time-dependent density functional theory

3.00 – 3.30pm: **Tim Zuehlsdorff**, Oregon State University, *Modeling nonadiabatic effects in linear optical spectra of complex systems using TDDFT*

3.30 – 4.00pm: TDDFTea and Coffee

4.00 – 4.30pm: **Vojtech Vlcek,** University of California Santa Barbara
Quasiparticle dynamics in and out-of equilibrium

4.30 – 5.00pm: **Xavier Andrade,** Lawrence Livermore National Lab,
The INQ Code, a State of the Art Implementation of TDDFT

7 - 9:30pm, Workshop Dinner, RBG Great Hall, 15 Washington St.

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Friday July 7

8.00am—8.40am Breakfast

8.45—9.15am: **Adrienn Ruzsinszky,** Temple University
Linear response in space and time, with application to symmetry breaking

9.15am – 9.45am: **Jefferson Bates**, Appalachian State, *Irreducible Polarization in the Hubbard Dimer: Exploring a Many-Body Concept with TDDFT*

9.45 – 10.15am: **Jianwei Sun**, Tulane University, *DFT error origins in open-shell d- and f-electron compounds revealed from SCAN's performance: self-interaction error, strong correlation, or both?*

10.15 – 10.45am: TDDFTea and Coffee

10.45 – 11.15am: **Stephan Kümmel** , University of Bayreuth
The Kohn-Sham current density - not real, but useful

11.15 – 11.45pm: **John Perdew,** Temple University
Symmetry Breaking: DFT and TDDFT Perspectives

11.45—2pm: Lunch

2.00 – 2.30pm: **Basile Curchod,** Unviersity of Bristol, *Driving new developments in excited-state molecular dynamics through challenging photochemical applications*

2.30 – 3.00pm: **Angel Rubio,** MPI Hamburg, *Quantum electrodynamics density functional theory (QEDFT): quantum light materials engineering*

3.00 – 3.30pm: **Attila Cangi,** CASUS Germany, *Electronic properties of matter under extreme conditions using time-dependent density functional theory*

3.30 – 4.00pm: TDDFTea and Coffee

4.00 – 4.30pm: **Lucia Reining,** Polytechnique, France
Perturbation theory: in what should we expand, and how?

4.30 – 5.00pm: **Roi Baer,** Hebrew University of Jerusalem
Stochastic vector methods in electronic structure

5.30 – 7.00pm: ***Poster Session***

Saturday July 8

8.00am—8.40am Breakfast

8.45—9.15am: **Will Glover**, New York University Shanghai, *Modeling photoexcited-charge transfer in complex systems with polarizable embedding*

9.15am – 9.45am: **Shaama Sharada,** University of Southern California
Catalyst discovery for metal-free photoredox CO2 reduction

9.45 – 10.00am: Student talk – **Thomas Trepl**, University of Bayreuth, *Real-Time Ehrenfest TDDFT as a Tool to Understand Light-Harvesting*

10.00 – 10.15am: Student talk – **Etienne Palos**, U. California, San Diego,
Postmodern DFT and Many-Body Interactions in Aqueous Phase Chemistry

10.15 – 10.45am: TDDFTea and Coffee

10:45 – 11.15am: **Michele Pavanello,** Rutgers University
Time-Dependent Orbital-Free DFT Unleashed

11.15—1:30pm: Lunch

1.30 – 2.00pm: **Eunji Sim**, Yonsei University, Korea
Density-corrected DFT applied to large systems

2.00 – 2.30pm: **Stefan Vuckovic**, Saarland University, *Near CCSD(T) Accuracy for Non-Covalent Interactions at Near DFT Cost*

2.30 – 3.00pm: **Filipp Furche,** University of California Irvine
Symmetries in Self-Consistent Field Response Theory

3.00 – 3.30pm: TDDFTea and Coffee

4.00 – 4.30pm: **Aurora Pribram-Jones**, University of California Merced
Examining time dependence in ensembles

4.30 – 5.00pm: **Neepa Maitra,** Rutgers Newark
HJK Couplings in TDDFT