

TDDFT School and Workshop at Rutgers Inn: Workshop Schedule, Aug 11—14, 2019

Sunday August 11

7.45am—8.40am Breakfast

8.45—8.55am: Opening Remarks

8.55 – 9.35am: **Christine Isborn**

Optical spectroscopy in the condensed phase

9.35 – 10.15am: **Ken Lopata**

Simulating Attosecond Dynamics and Observables with TDDFT

10.15 – 10.45am: TDDFTea and Coffee

10.45 – 11.25am: **John Herbert**

The hydrated electron

11.25 – 12.05pm: **Will Glover**

TBD

12.05—2pm: Lunch

2.00 – 2.40pm: **Jeff Neaton**

*Comparing TDDFT with *ab initio* many-body perturbation theory for excited states of solids*

2.40 – 3.20pm: **Filipp Furche**

Multi-state nonadiabatic molecular dynamics using TDDFT

3.20 – 3.50pm: TDDFTea and Coffee

3.50 – 4.30pm: **Alexey Akimov**

Nonadiabatic Molecular Dynamics with Δ SCF Excited States

4.30 – 5.10pm: **Sharon Hammes-Schiffer**

Multicomponent TDDFT: Integrating Electronic and Vibrational Excitations

Monday August 12

7.45am—8.40am Breakfast

8.45—9.25am: **Neepta Maitra**

Going beyond the adiabatic approximation – and coming back again

9.25am – 10.05am: **Carsten Ullrich** *TDDFT vs many-body approaches for excitons: long-range corrected xc kernels and screened exact exchange*

10.05 – 10.45am: **Junhyeok Bang**

Carrier Multiplication in Graphene Nanoribbons

10.45 – 11.10am: TDDFTea and Coffee

11.10 – 11.50am: **Michael Walter**

Accurate photoelectron properties from (time-dependent) DFT

11.50 – 12.30pm: **Kalman Varga**

TBD

12.30—2pm: Lunch

2.00 – 2.40pm: **Xavier Andrade**

TBD

2.40 – 3.20pm: **Matteo Gatti** *The connector theory approach: new approximations for exchange-correlation and materials design*

3.20 – 3.50pm: TDDFTea and Coffee

3.50 – 4.30pm: **Aurora Pribram-Jones**

New Approaches to Temperature-Dependent Approximations in (TD)DFT.

4.30 – 5.10pm: **Emmanuel Fromager**

Unified ensemble DFT for charged and neutral excitations

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Tuesday August 13

7.45am—8.40am Breakfast

8.45—9.25am: **Andre Schleife**

Femto-second charge dynamics and electronic stopping in self-irradiated silicon

9.25am – 10.05am: **Andrew Baczewski**

Transport properties in the warm dense regime

10.05 – 10.45am: **Benedetta Mennucci**

TDDFT and Excited states in biosystems: a successful marriage?

10.45 – 11.10am: TDDFTea and Coffee

11.10 – 11.50am: **Sahar Sharifzadeh**

Calculating the Optical Absorption Spectrum of Stacked Chromophores by a Combination of First-Principles TDDFT and Molecular Dynamics

11.50 – 12.30pm: **Christine Aikens**

Luminescence and real-time electron dynamics in gold and silver nanoparticles

12.05—2pm: Lunch

2.00 – 2.40pm: **Peter Elliott**

Ultrafast Spin Dynamics using Real-Time TDDFT

2.40 – 3.20pm: **John Perdew**

TBD

3.20 – 5.15pm: **Poster Session**

Wednesday August 14

7.45am—8.40am Breakfast

8.45—9.25am: **Bryan Wong**

A Primer on Real-Time TDDFT for Periodic Systems

9.25am – 10.05am: **Niri Govind**

Exploring Valence and X-ray Spectroscopies with Real-Time and Linear-Response TDDFT: Excited State Absorption & X-ray Emission

10.05 – 10.25am: **Student Prize Talk**

TBD

10.25 – 10:45am: TDDFTea and Coffee

10:45 – 11.25am: **Alberto Castro**

Ehrenfest dynamics, in & out of equilibrium

11.25 – 11.45pm: **Student Prize Talk**

TBD

11.45 – 12.25pm: **Michele Pavanello**

Mean field methods for ground and excited states with multireference character.

12.25 – 12.35pm: **Closing Remarks**

12.35—2.00 pm: Lunch