

International Symposium on  
**Ab Initio Electron Dynamics Simulations**

November 14-16, 2018

International Congress Center EPOCAL TSUKUBA

## November 14 (Wednesday)

8:30 – Registration

[Chair: Tomohito Otobe]

9:10 – 9:20 Opening (Kazuhiro Yabana)

9:20 – 10:00 **Kieron Burke**

University of California, Irvine

“Understanding TDDFT with the Hubbard dimer”

10:00 – 10:40

**John J. Rehr**

University of Washington

“Exchange and correlation in real-time and finite-temperature TDDFT”

Break

[Chair: Eric Suraud]

11:10 – 11:50

**Lin-Wang Wang**

Lawrence Berkeley National Laboratory

“Fast real time TDDFT and non-adiabatic molecular dynamics with detailed balance and dephasing”

11:50 – 12:30

**Guanhua Chen**

University of Hong Kong

“Time-dependent density functional theory for open systems and its applications”

Lunch Break

[Chair: Shiwu Gao]

14:00 – 14:40

**Sheng Meng**

Institute of Physics, Chinese Academy of Sciences

“Emergence of new states in photoexcited solids”

14:40 – 15:10

**Junhyeok Bang**

Korea Basic Science Institute

“Dephasing-induced ultrafast charge transfer in van der Waals heterostructures”

Break

[Chair: Kalman Varga]

- 15:40 – 16:20    **Eric Suraud**  
Paul Sabatier University  
“On the inclusion of dissipative effects in clusters and molecules”
- 16:20 – 16:50    **Kazuyuki Watanabe**  
Tokyo University of Science  
“Electron emission from nano carbon induced by laser irradiation, plasmon excitation and electron impact”
- 17:00 – 18:30    Poster session (with drinks and snacks)

## November 15 (Thursday)

- 8:30 – Registration  
[Chair: Sheng Meng]
- 9:00 – 9:40 **Everhard K.U. Gross**  
Max Planck Institute of Microstructure Physics  
“Laser-induced spin dynamics in solids: Some predictions from real-time TDDFT”
- 9:40 – 10:10 **Noejung Park**  
Ulsan National Institute of Science and Technology  
“Ab initio study of ultrafast spin dynamics of spin-orbit coupled semiconductor under the influence of circularly-polarized external fields”
- Break  
[Chair: George F. Bertsch]
- 10:40 – 11:10 **Simone Latini**  
Max Planck Institute for the Structure and Dynamics of Matter  
“Ab-initio exciton-polaritons: Cavity control of dark excitons in two-dimensional materials”
- 11:10 – 11:40 **Hirohiko Kono**  
Tohoku University  
“Multiconfigurational theories for the dynamics of molecules in intense laser fields: Anisotropic ionization of CO and structural deformation of C<sub>60</sub>”
- 11:40 – 12:10 **Takeshi Sato**  
University of Tokyo  
“Time-dependent wavefunction-based methods for intense laser-driven multielectron dynamics”
- Lunch Break  
[Chair: John J. Rehr]
- 13:30 – 14:00 **Yasushi Shinohara**  
University of Tokyo  
“Electron dynamics simulation for solid-state high-harmonic generation based on first-principles theory”

- 14:00 – 14:20     **Shi-Qi Hu**  
Institute of Physics, Chinese Academy of Sciences  
“Strong field induced even order high harmonic generation in graphene”
- 14:20 – 14:40     **Isabella Floss**  
Vienna University of Technology  
“Accounting for decoherence in solid-state TDDFT”
- 14:40 – 15:10     **Hannes Huebener**  
Max Planck Institute for the Structure and Dynamics of Matter  
“Floquet analysis of excitations in solids”
- Break (Conference Photo)
- [Chair: Yoshiyuki Miyamoto]
- 15:40 – 16:20     **Kalman Varga**  
Vanderbilt University  
“Volkov basis for simulation of interaction of strong laser pulses and solids”
- 16:20 – 17:00     **Shiwu Gao**  
Beijing Computational Sciences Research Center  
“Tunable spin and water transport through graphene nano channels”
- 18:00 – 20:00     Banquet at restaurant ESPOIR, 1st floor, EPOCAL Tsukuba

## November 16 (Friday)

- 8:30 – Registration  
[Chair: Lin-Wang Wang]
- 9:00 – 9:40 **Thomas A. Niehaus**  
Claude Bernard University Lyon 1  
“Electron dynamics from approximate time-dependent density functional theory”
- 9:40 – 10:20 **Yosuke Kanai**  
University of North Carolina at Chapel Hill  
“Electronic stopping from non-equilibrium real-time TDDFT simulation: Development and applications”
- Break  
[Chair: Guanhua Chen]
- 10:50 – 11:20 **Xavier Andrade**  
Lawrence Livermore National Laboratory  
“Calculation of non-linear electrical and thermal conductivity with real-time TDDFT”
- 11:20 – 11:50 **Kenji Iida**  
Institute for Molecular Science  
“Photoinduced electron dynamics of heterointerface systems simulated by massively parallel calculations”
- 11:50 – 12:10 **Shunsuke Yamada**  
University of Tsukuba  
“Microscopic and macroscopic descriptions for interaction of ultrashort light pulse with thin materials”
- Lunch Break  
[Chair: Yosuke Kanai]
- 13:30 – 14:00 **Yoshiyuki Miyamoto**  
Institute of Advanced Industrial Science and Technology  
“Thermal and non-thermal laser-induced lattice dynamics examined by TDDFT”

- 14:00 – 14:20 **Lei Yan**  
University of Tokyo  
“Plasmon-induced ultrafast hydrogen production in liquid water”
- 14:20 – 14:50 **Tomohito Otobe**  
Kansai Photon Science Institute  
“Laser-solid interaction in non-perturbative regime”
- [Chair: Everhard K.U. Gross]
- 15:20 – 15:50 **Mitsuharu Uemoto**  
University of Tsukuba  
“Maxwell+TDDFT ab initio multi-scale simulation and application to nano-optics”
- 15:50 – 16:10 **Atsushi Yamada**  
University of Tsukuba  
“Maxwell + nonadiabatic ab initio MD multi-scale simulation and application to impulsive stimulated Raman scattering spectroscopy”
- 16:10 – 16:30 **George F. Bertsch**  
University of Washington  
“Summary”

## Poster presentations

P – 1

**Srijana Bhandari**

Kent State University

“Fundamental gaps of condensed-phase organic semiconductors from single-molecule polarization-consistent optimally-tuned screened range-separated hybrid functional”

P – 2

**Daeho Han**

Ulsan National Institute of Science and Technology

“Orbital-based surface hopping dynamics with decoherence”

P – 3

**Ken Horikawa**

University of Tsukuba

“Length versus velocity gauge calculation for electron dynamics in crystalline solids”

P – 4

**Mehmet Emin Kilic**

Yonsei University

“Interface effects on the ionic conductivity of doped Ceria–Yttria-stabilized zirconia heterointerface”

P – 5

**In Seong Lee**

Ulsan National Institute of Science and Technology

“Decoherence induced surface hopping dynamics based on exact factorization and its applications”

P – 6

**Chang Woo Myung**

Ulsan National Institute of Science and Technology

“X-ray absorption fine structure spectra of single Pt on N-doped coronene”

P – 7

**Masashi Noda**

University of Tsukuba

“Direct wave vector excitations of silicon induced by optical near fields”

P – 8

**Shota Ono**

Gifu University

“Semiclassical derivation of the Rothwarf-Taylor model for quasiparticle and phonon dynamics in superconductors”



P – 9

**Dongbin Shin**

Ulsan National Institute of Science and Technology

“Enhancement of the 2nd order responses of insulators through a Berry curvature engineering”

P – 10

**Suhwan Song**

Yonsei University

“Correction abnormal DFT calculation via density correction”

P – 11

**Takashi Takeuchi**

University of Tsukuba

“Optical properties of metallic nanoparticle arrays calculated by SALMON”

P – 12

**Mitsuharu Uemoto**

University of Tsukuba

Spatio-temporal analysis of nonlinear optical responses by time-dependent density functional theory

P – 13

**Atsushi Yamada**

University of Tsukuba

“First-principles electron dynamics simulation study of high intensity laser irradiation on crystal systems: Pulse frequency dependent energy transfer”

P – 14

**Shengjie Zhang**

Institute of Physics, Chinese Academy of Sciences

“Laser induced magnetization in monolayer MoS<sub>2</sub>”