

# Workshop on Frontiers in Excited State Electronic Structure Methods: from Spectroscopy to Photochemistry



**16 - 19 May 2023**  
**An ICTP meeting**  
**Trieste, Italy**

Further information:

<http://indico.ictp.it/event/10170/>  
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A vast ecosystem of electronic structure methods and software populate the theoretical and computational scientific landscape. Excited state applications in solids and molecules are amongst the most employed ones, spreading from physics to chemistry to biology and beyond. However, the accurate modeling of excited state properties in realistic systems remains an open-challenge due to the complexity of the underlying electronic structure.

This workshop will gather code developers from several electronic structure packages (Quantum Espresso, Orca, DFTB+, Li<sup>+</sup>, SIESTA, Newton-X, Yambo, BigDFT, Onetep, SHARC, Octopus, etc) involved in excited state method developments and applications. We will focus our discussions on practical challenges, implementation bottlenecks, state-of-the-art methodological developments, as well as limitations in real systems applications.

A balanced audience of varied expertise (Post-Hartree-Fock, TDDFT, GW, Bethe-Salpeter, Excited State Adiabatic and non-Adiabatic dynamics) and working on diverse implementations (e.g. Gaussian basis, plane-waves, wavelets), will provide a fertile environment for exchanging ideas, sharing and comparing common problems and possible solutions, and exposing researchers working in the field to the variety of novel developments and features these codes have to offer.

## Topics:

- Light-Matter Interactions
- Spectroscopic characterization of excited states
- Ultrafast spectroscopy for excitation dynamics
- Charge separation and transfer
- Relaxation processes
- Adiabatic and non-adiabatic excited state dynamics
- Post-Hartree-Fock methods
- Time Dependent Density Functional Theory
- GW, Bethe-Salpeter and many-body perturbation methods
- Machine learning for excited states
- Quantum/Classical methods for ultrafast photoinduced dynamical processes

*Applicants are encouraged to submit an abstract for a poster presentation.*

## How to apply:

Online application:  
<http://indico.ictp.it/event/10170/>

Female scientists are encouraged to apply.

## Grants:

A limited number of grants are available to support the attendance of selected participants, with priority given to participants from developing countries. There is no registration fee.

## Directors:

U. MORZAN, ICTP, Italy  
M. STELLA, ICTP, Italy  
V. VITALE, UniTS, Italy

## Local Organiser:

R. GEBAUER, ICTP, Italy

## Workshop Speakers:

J. BLUMBERGER, University College London, UK  
F. BONAFÉ, Max Planck Institute for the Structure and Dynamics of Matter, Germany  
I. CARNIMEO, SISSA, Italy  
B. CURCHOD, University of Bristol, UK  
S. FERNÁNDEZ ALBERTI, National University of Quilmes, Argentina  
N. FOGLIA, Max-Planck-Institut für Kohlenforschung, Germany  
L. GONZALEZ, University of Wien, Austria  
M. GONZÁLEZ LEBRERO, University of Buenos Aires, Argentina  
N. HINE, University of Warwick, UK  
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P. PAVONE, University of Humboldt, Germany  
L. RATCLIFF, University of Bristol, UK  
L. REGO, University of Santa Catarina, Brazil  
A. REILY ROCHA, University of Sao Paulo, Brazil  
C. SANCHEZ, University of Cuyo, Argentina  
D. SCHERLIS, University of Buenos Aires, Argentina  
A. TROISI, University of Liverpool, UK  
D. VARSANO, CNR, Italy

## Deadlines:

**16 March 2023**

for applicants requesting financial and/or visa support

**1 May 2023**

for all other applicants



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