# Workshop on "Advances in electronic structure theory"

27-29 April 2015, UPMC, Jussieu Campus, Amphi Charpak (Tower 22, street level), Paris

*https://wiki.lct.jussieu.fr/workshop*

## Monday 27 April

***Chair: Paola Gori-Giorgi***

9:00 – 9:30 **Paul Ayers**, *A mean-field description of strong correlation using antisymmetric products of interacting geminals*

9:30 – 10:00 **Garnet Chan**, *Dynamical correlation in multireference problems*

10:30 – 10:30 **Gustavo Scuseria**, *A quantum chemistry view of the strong correlation problem*

**10:30 – 11:00 Coffee break**

***Chair: Peter Reinhardt***

11:00 – 11:30 **Hermann Stoll**, *Filling the gap between pseudopotential and all-electron schemes*

11:30 – 12:00 **Trond Saue**, *Electron correlation in a relativistic perspective*

**12:00 – 14:00 Lunch at "L'Ardoise" near Tower 25 (for all participants)**

***Chair: Kimihiko Hirao***

14:00 – 14:30 **Hans Jørgen Jensen**, *Status and perspectives for multiconfiguration short-range density functional theory*

14:30 – 15:00 **Emmanuel Fromager**, *State-averaged multi-determinant density-functional theory based on ensembles and range separation*

15:00 – 15:30 **Eleonora Luppi**, *Describing the electron dynamics with TD-CI an AO basis: the case of high-harmonic generation spectroscopy H atom and molecule*

**15:30 – 16:00 Coffee break**

***Chair: Julien Toulouse***

16:00 – 16:30 **Irek Grabowski**, *Orbital-dependent second-order scaled-opposite-spin correlation functional in the optimized effective potential method*

16:30 – 17:00 **Andy Teale**, *Towards simple density-functional approximations from accurate ab initio theory*

17:00 – 17:30 **Tomasz Wesolowski**, *The issue of orthogonality in frozen-density embedding theory*

## Tuesday 28 April

***Chair: Janos Angyan***

9:00 – 9:30 **Kieron Burke**, *Systematic approach to density functional approximations*

9:30 – 10:00 **Weitao Yang**, *Fractional perspectives of DFT and local scaling corrections*

10:30 – 10:30 **Kasia Pernal**, *A computationally efficient geminal-based method for accurate description of chemical systems*

**10:30 – 11:00 Coffee break**

***Chair: Bernard Silvi***

11:00 – 11:30 **Carlo Adamo**, *An overview on parameter-free double hybrids*

11:30 – 12:00 **Memorial Ziegler**

**12:00 – 14:00 Lunch at "L'Ardoise" near Tower 25 (for all participants)**

***Chair: Evert Jan Baerends***

14:00 – 14:30 **Hardy Gross**, *Conditional probability amplitudes for electrons and nuclei*

14:30 – 15:00 **Robert van Leeuwen**, *The density to potential mapping in time-dependent density-functional theory*

15:00 – 15:30 **Mark Casida**, *Challenge of time-dependent density-functional theory for photochemistry*

**15:30 – 16:00 Coffee break**

***Chair: Lucia Reining***

16:00 – 16:30 **Neepa Maitra**, *Dynamics of charge-transfer in time-dependent density functional theory*

16:30 – 17:00 **Carsten Ullrich**, *Towards nonempirical hybrid functionals for excitonic properties in solids*

17:00 – 17:30 **Matteo Gatti**, *Dynamical screening: plasmons, excitons and photoemission satellites*

## Wednesday 29 April

***Chair: Roberto Dovesi***

9:00 – 9:30 **Cyrus Umrigar**, *Ground-state quantum Monte Carlo methods and the sign problem*

9:30 – 10:00 **Ali Alavi**, *Calculation of pure expectation values and properties from FCIQMC*

10:30 – 10:30 **Michel Caffarel**, *Fixed-Node Diffusion Monte Carlo with CI-type trial wave functions*

**10:30 – 11:00 Coffee break**

***Chair: Esmaïl Alikhani***

11:00 – 11:30 **Claudia Filippi**, *Quantum Monte Carlo for excited-state calculations in complex environments*

11:30 – 12:00 **Peter Gill**, *Using Quantum Monte Carlo and wave function methods to improve density functional theory*

**12:00 – 14:00 Lunch at "L'Ardoise" near Tower 25 (for all participants)**

***Chair: Jean-Philip Piquemal***

14:00 – 14:30 **Yvon Maday**, *Some elements of analysis for Andreas' systematic way to correct density functional approximations*

14:30 – 15:00 **Elisa Rebolini**, *Calculating excitation energies along the range-separated adiabatic connection*

15:00 – 15:30 **Mathieu Lewin**, *On the Lieb-Oxford inequality: best constant, gradient correction and the homogeneous electron gas*

**15:30 – 16:00 Coffee break**

***Chair: Olivier Parisel***

16:00 – 16:30 **Bastien Mussard**, *Range-separated random-phase approximations*

16:30 – 17:00 **Trygve Helgaker**, *DFT in magnetic fields*