Miniworkshop REST in Paris

Common problems and solutions in core and valence theoretical spectroscopies

Thursday 7 December: Invited talks (Amphi Charpak, RC or SB floor, patio 23-32)

Chair: Ch. Brouder

8:30	9:00	Registration
9:00	9:30	**Amélie Juhin** *Welcome and introduction to spectroscopies*
9:30	10:30	**Guillaume Radtke** *Standard approaches for core level spectroscopies. From single particle to multielectronic methods*
10:30	11:00	Coffee Break
11:00	11:45	**Francesco Sottile** *Introduction to standard methods for valence spectroscopies*
11:45	12:30	**Jianqiang Zhou** *Photoemission spectroscopy from first principles*
12:30	14:00	Lunch at the Mineral Collection of IMPMC/UPMC (Patio 25-14)

Chair: M. Gatti

14:00	14:45	**Pierluigi Cudazzo** *Cumulant expansion of the electronic polarizability: beyond the static Bethe-Salpeter equation*
14:45	15:45	**Yves Joly** *From DFT to time-dependent DFT*
15:45	16:15	Coffee Break
16:15	17:15	**Maurits Haverkort** *When and why do we need multi-configurational methods in spectroscopy whereas mean-field approaches work for the ground state of the same material?*
17:15	18:00	**Christian Brouder** *The challenge of optical spectra calculations: the unsolved problem of the color of materials*

Friday 8 December: Contributed talks (Amphi Charpak, RC or SB floor, patio 23-32)

Chair: Y. Joly

8:45	9:10	**Frank de Groot** *Calculating x-ray emission and fluorescence yield*
9:10	9:35	**Ondřej Šipr** *Finite lifetime broadening of calculated x-ray absorption spectra: possible artifacts close to the edge*
9:35	10:00	**Javier Fernandez-Rodriguez** *Electronic structure of greigite (Fe_3S_4) derived from the XMCD spectra*
10:00	10:30	Coffee Break

Chair: J. Rehr

10:30	10:55	**Christian Vorwerk** *All-electron many-body approach to core excitations in solids*
10:55	11:20	**Igor Reshetnyak** *Optical properties of vanadates: an accurate theoretical description*
11:20	11:45	**Lorenzo Sponza** *Exciton interference in hexagonal boron nitride*
11:45	13:45	Lunch break + Poster session (room 401, 4th flour, corridor 22-23)

Chair: Ph. Sainctavit

13:45	14:10	**Anu Baby** *Lattice mismatch drives spatial modulation of corannulene tilt on Ag(111)*
14:10	14:35	**Ivan Radovic** *Theoretical modeling of experimental EELS data for freestanding and supported graphene*
14:35	15:00	**Vita Ilakovac** *RIXS probes the electron-phonon coupling in the spin-liquid μκ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$*
15:00	15:30	Coffee Break

Chair: F. Sottile

15:30	15:55	**Emmanuel Fromager** *Direct extraction of exact individual excited-state energies from (time-independent) ensemble density-functional theory*
15:55	16:20	**Sergey Bokarev** *Theoretical soft X-ray spectroscopy of transition metal compounds: A multi-reference wave function approach*
16:20	16:45	**Emmanuelle de Clermont Gallerande** *Modeling of X-ray Raman Spectroscopy: The core-hole and core–wave function issue in the single-particle*

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Friday 8 December (lunch time): Contributed posters (room 401, corridor 23-22, 4th floor)

Mathieu Chassé
Ab-Initio Modelling of Scandium K-edge XANES Spectra

Killian Deur
Direct extraction of individual state energy from the ensemble energies: Application in the no symmetric Hubbard dimer

Javier Fernandez-Rodriguez
Multiplet calculations with the XCLAIM code

Jurij Galanzew
Electronic Structure Studies of Thorium Systems

Cairedine Kalai
Combining Density-functional Theory And Wave-function Methods: The RSλH + MP2 Scheme

Laurent Mazouin
Green functions in site-occupation embedding theory

Solène Oberli
Time-dependent quantum description of molecular double core hole states: vibrationally resolved photoelectron spectra of CO

Julien Paquier
Relativistic range-separated density-functional theory

Abhilash Ravikumar
Electronic and magnetic properties of core-excited organic molecules on hybrid graphene interfaces

Bruno Senjean
Site occupation embedding theory

Petra Votavová
Fano-CI method for decay widths of metastable excited states of atomic and molecular systems