

	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
	Session 1: Electronic structure methods	Session 2: Optical properties of materials	Session 3: Vibrational properties of materials	Session 4: Strongly correlated systems	Session 5: Quantum computing*
9:30-10:00	Registration + Welcome talk				
10:00 - 11:00	M. Mayorga <i>Is there any recipe for using RPA?</i>	Y. Liu (online) Calculations of absorption tail in mixed halide perovskite	M. Kotiuga <i>Insights from vibrational properties in determining structural prototypes of ferroelectrics</i>	M. Chatzieftheriou <i>Metal-insulator transitions in the Hubbard model: local vs non-local correlation effects</i>	X. Bonet-Monroig <i>Quantum computing: why should I (and you) care?</i>
11:00- 11:30	A. El Sahili <i>Beyond GW:non-unique method and diversity of choices</i>	H. Fried <i>Calculation of optical signatures of defects: comparing different methods</i>	A. Castellano <i>Mode-coupling theory anharmonic lattice dynamics</i>	B. Chatterjee <i>Ground state symmetries collective modes in TA2NiSe5 - an excitonic insulator candidate</i>	C. Emeis <i>Electron-plasmon satellites in the spectral function of highly-doped HfS2</i>
11:30 - 12:00	COFFEE BREAK	COFFEE BREAK	COFFEE BREAK	COFFEE BREAK	COFFEE BREAK
12:00 - 12:30	M. Gunes <i>Charge density as a functional of the potential: Connector theory approach</i>	L. Biancorosso <i>Plasmon-assisted electron dynamics in photocatalysis: hydrogen production from formic acid</i>	J. Batista <i>Machine learning assisted calculation of phonon properties in layered hBN</i>	A. Carrasco Alvarez <i>Charge ordering as the driving mechanism for superconductivity in rareearth nickel oxides</i>	D. Corona <i>Encapsulated BN nanocages and nanocapsules as anode materials for magnesium-ion batteries: A DFT study</i>
12:30 - 13:00	M. Sadegh Shakeri <i>Many-body GW calculation od X-ray absorption spectra of Cu0, Cu+, Cu2+ and Cu3+ structures</i>	M. Marino <i>Ab initio study of Fe-phthalocyanine adsorption on the antiferromagnetic NiO(001) surface</i>	M. Lezoualc'h <i>Charge density waves in 1T-VeS2</i>	A. Osorio <i>Understanding borophene: From the atomic structure to the electronic response</i>	
13:00 - 13:30	I. Mukatayev <i>Investigation of atomic core levels with ab initio many body theories</i>	S. Grillo <i>Non-trivial excitonic fingerprints and optical anisotropy of 2D Tellerium</i>	A. Custodio <i>Nitrogen-vacancy center: understanding the electronic structure from ab-initio calculations</i>	C. Morassut <i>Analysis and comparison of optimal-continuum Gaussian basis sets for high harmonic generation spectra for atoms and molecules</i>	END OF CONFERENCE

13:30 - 15:30	LUNCH BREAK	LUNCH BREAK	LUNCH BREAK	LUNCH BREAK	
15:30 - 16:30	A. Ammar <i>Transcorrelated Selected Configuration Interaction</i>	S. Canola <i>Molecular systems probed by near-field spectroscopy</i>	C. Verdi <i>Phonon anharmonicity in quantum paraelectrics beyond density-functional theory</i>	C. Yue <i>BStrong correlation and unconventional superconductivity in bulk and trilayer alkali-doped fullerides</i>	
16:30 - 17:00	Coffee break	Coffee break	Coffee break	Coffee break	
17:00 - 17:30	L. Urquiza <i>Pseudopotential Bethe-Salpeter calculations for shallow-core spectra</i>	Vun Binh <i>Theoretical studies of novel graphene based nanostructures</i>	Y. Pan <i>Non-equilibrium dynamics of chiral valley phonons from the time-dependent Boltzmann equation</i>	What is the ETSF? Alberto Castro	
17:30 - 18:00	Y. Schmerwitz <i>Calculations of excited electronic states by converging on saddle points using generalized mode following</i>	Social event and Social dinner	Poster session	Industry session: Francesco Calcavecchia	
18:00 - 18:30	E. Selenius <i>Improving density functional calculations of intramolecular charge transfer excited states</i>				
18:00 - 19:30					
20:00					