YRM ETSF 2025

The 21st Young Researchers' Meeting

26-30 May 2025, Trieste, Italy.

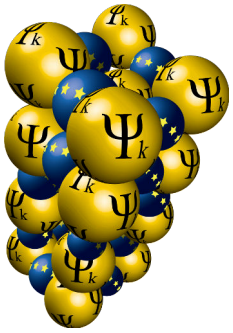
PROGRAM AND BOOK OF ABSTRACTS

cecam Centre Européen de Calcul Atomique et Moléculaire

ETSF

FERMI FÉDÉRATION DE RECHERCHE MATIÈRE ET INTERACTIONS

nanoX NANOSCALE SCIENCE AND ENGINEERING



Website and Contact

https://sites.google.com/view/yrm2025/home
You can contact us at yrm2025organizers@gmail.com.

Venue & Conference Room

SISSA – Scuola Internazionale Superiore di Studi Avanzati – was founded in 1978 and is a scientific center of excellence within the national and international academic scene. The SISSA campus is located in Opicina (Trieste), in Via Bonomea 265. It can easily be reached via public transportation, which connects the campus to downtown Trieste (at 4 km only), or via highway. Main options are taking the bus line 38 or tram 2. Tickets must be purchased beforehand at newsstands or tobacconists or tickets machines on Trieste streets and must be validated using the machines on the buses. There are single-run tickets, 10-run tickets or transit pass (biweekly, monthly, for the whole buses transport system). It's not possible to buy tickets on board. For more information on how to reach SISSA, please visit https://www.sissa.it/about/how-reach-us.

SISSA building may be entered through two entrances: main entrance on level 0 and a back entrance on level 2 (note that the back entrance requires badge access). From the main entrance, the venue (Room 005) is easily reached on the ground floor by walking straight forward past the reception desk. It may be found next to Room 004, visible as one enters through the main entrance. From the back entrance on the second floor, it's necessary to take the staircase or elevator to the ground floor, which may be accessed to either the left or right as one enters through the back entrance. Reaching the ground floor, one may find Room 005 in the area straight below the back entrance, next to the reception desk.

Hotels

Opera Figli del Popolo

Easily accessible from the city center and the Trieste train station, Opera Figli del Popolo is located at *Largo Papa Giovanni XXIII, 7, Salita dei Montanelli, 1/1*. To reach the conference from the hotel, you will need to tranfser to bus line 38 (through which passes by SISSA.

Le Terrazze

Located right at the city center, Le Terrazze is located at *Via Fabio Filzi, 21*. To reach the conference from the hotel, you will need to take the bus 38 which reaches SISSA in 15 minutes.

Organizers

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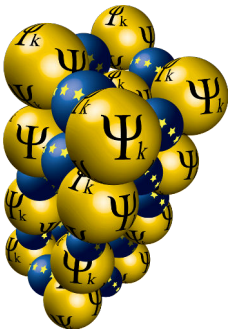

Detailed Program

	Monday	Tuesday	Wednesday	Thursday	Friday
	Electronic Structure and Method Development		Optical Properties of Materials	Strongly Correlated Systems and Magnetism	High Performance Computing
8:30 - 9:30	Registration & Welcome Talk				
9:30 - 10:30	**Tommaso Nottoli**	**Maryam Azizi**	**Marta Monti**	**Francesca Paoletti**	**Aleksandar Zivkovic**
10:30 - 10:55	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
10:55 - 11:20	Flash presentations	Advancing Photoemission Spectra Analysis with Three-Body Green's Function Formalism **Emma Nogué**	Computational and Experimental Investigation of Curcumin Derivatives as Potential Photosensitizers for Photodynamic Therapy **Ali Ghiami-Shomami**	Extended Hubbard functionals insight on transition-metal oxides for sodium-ion batteries **Domenico Corona**	Exploiting Parallelism for Fast Feynman Diagrammatics **John Sturt**
11:20 - 11:45	Computing the one-body reduced density matrix with Quantum Monte Carlo for solids **Carlos Rodriguez Perez**	Exploring superconducting nickelates electronic structures with the *GW* approximation **Jean-Baptiste de Vaulx**	Finite momentum excitons in scintillating materials and their implications for dark matter-electron scattering **Nora Taufertshöfer**	Bouncing-ball quantum scars in two-dimensional systems **Simo Selinummi**	**Fabio Caleffi** Industry session
11:45 - 12:10	First-principles study of Bi(trimer) on a Ge(111) surface **Montserrat Navarro Espino**	Simulations of the Thorium Nuclear Clock **Martin Pimon** Vibrational Properties of Materials and Transport	Optical properties of anisotropic excitons in GeS **Mehdi Arfaoui**	Revealing spinons by proximity effect **Antonio Maria Tagliente**	
12:10 - 13:40	Lunch break	Lunch break	Lunch break	Lunch break	Closing remarks
13:40 - 14:40	**Abdallah El Sahili**	**Ivan Maliyov (online)**	**Elisa Serrano Richaud**	**Pauline Besserve**	**End of Conference**
14:40 - 15:05	Benchmark study of many-body methods for the prediction of band alignment at hetero-interfaces, using 1D Hubbard models **Jean Goossaert**	Scartronics: Boosting Quantum Transport in Two-Dimensional Systems with Variational Scarring **Fartash Chalangari**	Optical Absorption in Indirect Semiconductor to Semimetal PtSe2 Arises from Direct Transitions **Sabrine Ayari**	Local classical correlations between physical electrons **Gabriele Bellomia**	
15:05 - 15:30	Coffee break	Coffee break	Coffee break	Coffee break	
15:30 - 15:55	Temperature dependence of band gaps of inorganic halide perovskites **Milan Jocic**	From Symmetry to Stability: Structural and Electronic Transformation in Cs2KInI6 **Mohammad Bakhsh**	Unveiling the Role of Electron-Phonon Scattering in High-Order Harmonics **Thomas Lettau**	Altermagnetism from interaction-driven itinerant magnetism **Samuele Giuli**	
15:55 - 16:20	From single bond to line defects: a case study from a novel two-dimensional network-forming material **Marco Dirindin**	Structural phase transitions in monolayer TMDs with a neural-network interatomic potential **Davide Bidoggia**	Electronic properties of 2D Transition Metal Dichalcogenides : an ab initio study confirmed by experiment **Felana Andriambelaza**	**Social debate**	
16:20 - 16:45	**Social event** Hiking to Castelletto di Miramare (through Strada Napoleonica)	Chaotic dynamics creates and destroys branched flow **Esko Toivonen**	Sum frequency generation from real-time simulation in 2D crystals **Mike Pionteck**		
16:45 - 18:00		Coffee break & poster session			
18:00 - 20:00					
20:00 -				**Social dinner** **@ Suban**	

Temperature dependence of band gaps of inorganic halide perovskites

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Recently, halide perovskites have been praised for their low-cost and high performance capabilities. However, in order to give reliable and accurate predictions on their performance and stability using *ab-initio* methods, one should first provide an adequate description of their electronic structure.

Reasonably accurate band gaps can be obtained using conventional DFT with local or semi-local functionals but this is a result of error cancellation due to the neglect of spin-orbit coupling (SOC) effects. Using hybrid functionals with full SOC treatment still yields an underestimated value of the band gap. In order to get correct results of the band gap, temperature effects caused by electron-phonon interaction must also be included.

We propose a combination of DFT with hybrid PBE0 functional, combined with Allen-Heine-Cardona (AHC) method, and the evaluation of anharmonic phonon frequencies using self-consistent phonon method [1]. We also propose a way to account for energy level renormalization and broadening at the same time by utilizing a procedure based on self-consistent Migdal approximation. Obtained results for $CsPbX_3$ (X=Cl, Br, I) halide perovskite band gaps for bulk crystals cover a wide range of temperatures which can be compared with experimental data, as seen in Figure 1.

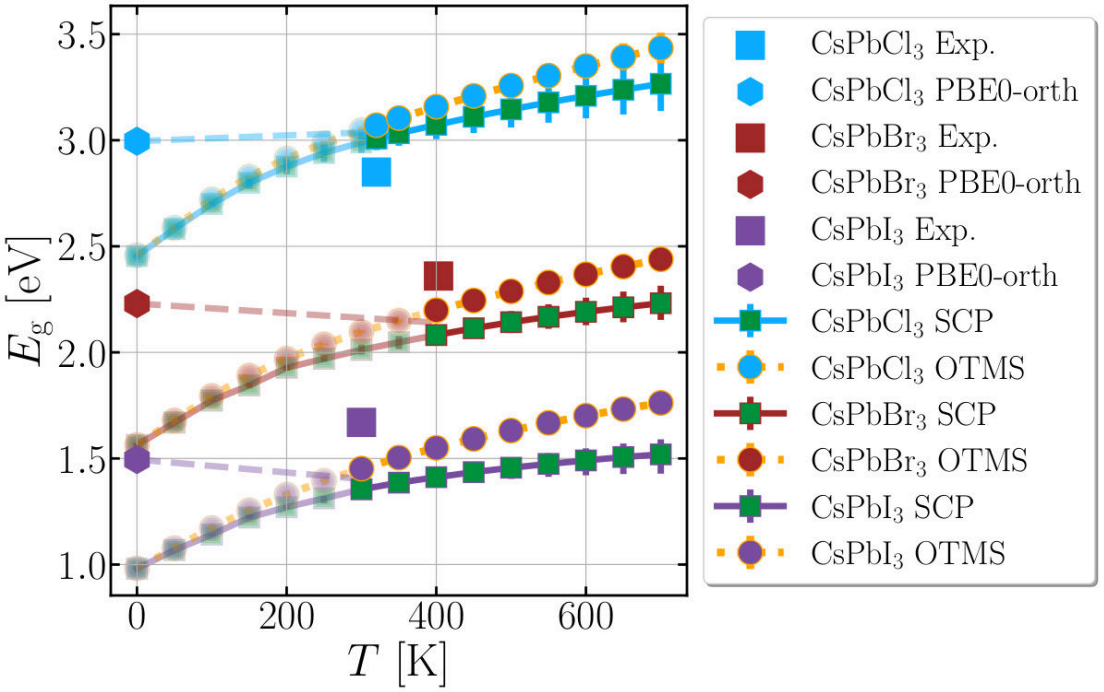

Figure 1: Band gaps of $CsPbX_3$ (X=Cl, Br, I) obtained using DFT with PBE0 hybrid functional and AHC correction for temperature effects compared with experimental values (disconnected squares). Results are obtained using on-the-mass-shell (OTMS) approximation (circles) and more refined self-consistent procedure (SCP) based on self-consistent Migdal approximation (connected squares). Zero temperature calculations were performed on an orthorhombic structure (hexagons), while temperature corrections were added on results with cubic phase. Lines and symbols at temperatures above (below) the formation of the cubic phase are shown as opaque (transparent) for each material.

References

[1] M. Jocić, N. Vukmirović, *Phys. Chem. Chem. Phys.* **25**, 29017 (2023).