



UNIMORE
UNIVERSITÀ DEGLI STUDI DI
MODENA E REGGIO EMILIA

Dipartimento di Scienze Fisiche,
Informatiche e Matematiche



FIM-S3 SEMINAR

Ab initio spectroscopy and high-throughput screening of complex materials

Monday February 17th, 2025 – 11.00 (sharp)

S3 Seminar Room, 3rd Floor, Physics building

Remote link: [Teams](#)

Speaker

Caterina COCCHI – Carl von Ossietzky Universität Oldenburg, Germany

Abstract

Semiconducting photocathode materials are crucial for developing next-generation particle accelerators, enabling ultrabright electron sources. Experimental challenges in synthesizing and characterizing these compounds demand complementary efforts from state-of-the-art computational methods [1]. In this seminar, I will demonstrate how cutting-edge theoretical approaches have significantly advanced our understanding of these materials. First, I will illustrate how ab initio spectroscopy techniques have provided invaluable insights into their electronic and spectroscopic properties, from the visible to the core level regions [2-6]. Second, I will discuss how the development of automated simulation protocols has enabled the discovery of novel compositions and crystalline phases within the established classes of alkali antimonides and tellurides [7-10].

References

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- [5] C. Cocchi, *Phys. Status Solidi RRL* **14**, 2000194 (2020).
- [6] J. Santana, H.-D. Saßnick, and C. Cocchi, *J. Phys. Mater.* **7**, 035004 (2024).
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- [10] R. Schier, D. Guo, H.-D. Saßnick, and C. Cocchi, *Adv. Theory Simul.* **7**, 2400680 (2024).
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Host: Elisa Molinari

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