

Friday Materials Science Colloquia #12

Friday, June 7th 2024, 12 p.m.
Seminar room, U5 Building – via Roberto Cozzi 55, Milano

Lecturer: **Aldo Ugolotti**

Title: Understanding the Ga₂O₃ growth on different substrates, towards the integration into Si-based devices.

Abstract:

Ga₂O₃ has attracted much attention in the field of power electronics, electronics for harsh environments and solar-blind sensors as a wide bandgap material with notable performances, due to one of the highest values of the breakdown voltage and of the Baliga figure of merit known among semiconductors[1-2].

However, experiments show that Ga₂O₃ possesses several metastable polymorphs which become competitive during the growth, throughout a vast combination of techniques and parameters. Therefore, a first part of this talk will be focusing onto the investigation of the growing mechanism of Ga₂O₃ α, κ and β phases on Al₂O₃. A model based onto the classical nucleation theory will be discussed, using recent ab-initio calculations[3] and experimental results from on-going collaborations with experimental groups.

For the development of next generation devices, the monolithic integration of Ga₂O₃ in the current Si-based technology is paramount. Nonetheless, the epitaxial growth of Ga₂O₃ on Si surfaces is undermined by several factors, such as a large misfit at the interface, the strong tendency of Si to oxidize, and the possibility to form a Ga-Si eutectic amalgam. In addition, several dangling bonds are expected at the interface, potentially undermining the overall quality of the growing film.

In order to start investigating such issues, the second part of the talk will be focused on the structure and electronic properties of two prototypical interfaces, namely Ga₂O₃/SiO_x/Si(100) and Ga₂O₃/3C-SiC(110). Through the comparison with pristine, bulk-like Ga₂O₃ some insights about the interface energy will be discussed.

[1] M. A. Mastro et al., ECS J. Solid State Sci. Technol. 6, P356 (2017)

[2] S. J. Pearton et al., J. Appl. Phys. 124, 220901 (2018)

[3] I. Bertoni et al., J Mat. Chem. C 12, 1820 (2024)

Lecturer: **Giorgio Tseberlidis**

Title: From Pycen Complexes to Kesterites: a journey from Catalysis to Photovoltaics and back

Abstract:

While seemingly distinct fields, catalysis and photovoltaics (PV) share several fundamental principles and characteristics. Both fields contribute to sustainable processes: efficient catalytic paths can lead to cleaner industrial processes while PV directly contribute to renewable energy generation by harnessing solar power. Moreover, both fields rely on advancements in material science and both strive for maximum efficiency.

Pycen metal complexes are coordination compounds formed by the binding of metal ions with Pycen macrocyclic ligands, known for their ability to form stable complexes with a variety of metal ions, often exhibiting high selectivity and strong coordination due to their cyclic and preorganized structure. Pycen metal complexes are successfully used as catalysts in a variety of chemical reactions such as nitro-aldol reaction, carbene transfer reaction, oxidations,

reductions, CO₂ fixation, as well as in electro-/photo- catalytic systems.[1] Similarly, kesterites, Cu₂ZnSn(S,Se)₄, known for their PV application as an emerging thin-film chalcogenide solar device technology, can find their application also as efficient photocatalyst in water splitting and water remediation. Kesterites show high cost-effectiveness thanks to low production costs, earth-abundance and non-toxicity of their composing elements. Their solution-based synthesis makes them suitable also for flexible and Product-Integrated PV (PIPV), making them an attractive alternative to silicon PV technologies.[2] Besides, their properties (such as energy gap, transparency, resistance, charge carrier density and mobility) can be tuned by partial or complete substitution of one or more components allowing their employment also in tandem solar architectures.[3] However, despite the promising efficiencies already reached, a complex phase diagram and a not-ideal device architecture inherited from former thin-film technologies and featuring CdS, prompt the scientific community to put efforts in kesterite solar cell optimization, especially for PIPV applications. Therefore, we have demonstrated how Atomic Layer Deposited (ALD) Zn_xSn_{1-x}O and TiO₂ can be reliable buffer layers, leading to Cd-free kesterite thin-film solar cells with results comparable to the CdS-containing reference devices.[4] Besides PV, recently we have experimentally demonstrated how kesterite nanoparticles can be an efficient photocatalyst in the degradation of emerging water micropollutants, doubling (in laboratory scale) the efficiencies currently registered in the industrial water treatment plants.

[1] N. Panza et al. Dalton Trans., 51, 10635-10657 (2022)

[2] G. Tseberlidis et al. Solar Energy, 208, 532–538 (2020)

[3] G. Tseberlidis et al. ACS Omega, 7, 23445–23456 (2022)

[4] G. Tseberlidis et al. ACS Materials Lett., 5, 219–224 (2023)