

**Department of Chemical Science and Technologies**  
**Aula Gismondi**  
**December 18<sup>th</sup> 2025**

**Third-Year Meeting**  
**MUR Excellence Program 2023–27**



## Dottorato Scienze Chimiche

9 Ozge Eslek ozge.eslek@uniroma2.it  
*Synthesis and Characterization of Photocurable, Smart and Semi-interpenetrated Hydrogels*  
Ozge Eslek, Fabio Domenici, Gaio Paradossi

10 Alessia Fata alessia.fata@students.uniroma2.eu  
*Synthesis of Iron-N-methyl corroles as chiral catalysts*  
Alessia Fata, Francesco Pizzoli, Roberto Paolesse, Sara Nardis

11 Agnese Foglietti agnese.foglietti@students.uniroma2.eu  
*Phase-change heterostructures based on MoSe<sub>2</sub> intercalated with Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub>*  
A. Foglietti, S. De Simone, S. Calvi, A. Díaz Fattorini, C. Petrucci, F. Arciprete, R. Calarco and M. Longo

12 Alessandro Iannini alessandro.iannini@uniroma2.it  
*Synthesis of Novel Organic Dyes for Light Driven Applications*  
Alessandro Iannini, Veronica Spinelli, Maria G. Iaquaniello, Lorenzo Tommasi, Valeria Conte, Federica Sabuzi and Pierluca Galloni

13 Jordy Alexis Lerma-Escalera jordyalexis.10@gmail.com  
*Programming transcription delay in cell-free systems*  
Jordy Alexis Lerma-Escalera, Juliette Bucci, Ana Urošević, Romain Amador, Gianfranco Ercolani and Francesco Ricci

14 Antonio Licheri Antonio.Licheri@uniroma2.it  
*Click Chemistry-Mediated Attachment of Spacers on Biochar: A Smart Tool for Robust and Reproducible Biosensing*  
Antonio Licheri, Veronica Mattarelli, Claudia Mazzuca, Silvia Orlanducci, Laura Micheli, Riccardo Salvio

15 Francesca Cosimina Miceli francesca.cosimina.miceli@uniroma2.it  
*MAIGRET: an antibody-responsive cell-free transcription system for CRISPR-based ultrasensitive immunoassay*  
Francesca Miceli, Sara Bracaglia, Daniela Sorrentino, Alessandro Porchetta, Simona Ranallo, Francesco Ricci

16 Miriam Quattrociocchi quattrociocchimiriam@gmail.com  
*Controlling in-vitro transcription through a DNA-based dimerization network*  
Miriam Quattrociocchi, Simone Brannetti, Erica Del Grosso, Francesco Ricci

17 Raffaella Salerno, Eleonora Bolli eleonora.bolli@cnr.it  
*Harnessing Nanodiamond Films for Photon-Enhanced Thermionic Emission*  
Raffaella Salerno, Alessandro Bellucci, Eleonora Bolli, Matteo Mastellone, Veronica Valentini, Riccardo Polini and Daniele Maria Trucchi

18 Sara Scalia

[sara.scalia@uniroma2.it](mailto:sara.scalia@uniroma2.it)

*Immune-induced antibody-DNA hybrid*

Sara Scalia, Marco Cappa, Lorenzo Rovigatti, Erica Del Grosso, Francesco Ricci

# eXpanding CHEMistry: implementing excellence in research and teaching

## X-CHEM III year Meeting

December 18<sup>th</sup> Department of Chemical Science and Technologies

*Tune, extend and narrow the useful dynamic range of cell-free transcription biosensors through programmable DNA-based stem-loop hairpin reporters*

João M. R. Aguiar,<sup>1</sup> Sara Bracaglia,<sup>1</sup> Simona Ranallo,<sup>1</sup> and Francesco Ricci <sup>1</sup>

<sup>1</sup> Department of Chemical Sciences and Technologies, University of Rome, Tor Vergata, Via della Ricerca Scientifica, 00133 Rome, Italy.

Email presenting author: aguiar@scienze.uniroma2.it

Cell-free transcription biosensors reporting systems are reliant on single-site biomolecular recognition which imposes an intrinsic limitation on the biosensor's dynamic range that spans approximately 81-fold.<sup>1</sup> Here, we present rational strategies to tune, extend, and narrow the dynamic range of cell-free transcription biosensing platforms. To do so, we engineered a set of optically labelled stem-loop DNA reporters whose dynamic range for detecting a specific RNA output can be precisely controlled by adjusting their switching equilibrium constant ( $K_S$ ). This straightforward approach enables the dynamic range of a model cell-free transcription biosensor to be programmed across more than 4 orders of magnitude. By combining DNA-based reporters with differing affinities, we further expanded the dynamic range of a cell-free transcription biosensor well beyond the conventional two orders of magnitude, achieving up to  $10^4$ -fold coverage. We also demonstrate the creation of two-step dynamic responses by mixing hairpin reporters with highly distinct affinities. Finally, integration of signaling and non-signaling stem-loop reporters allowed us to compress the dynamic range of this biosensor to as little as 3-fold, enabling heightened sensitivity for precise measurements. Overall, this modular framework enables the customization of cell-free transcription biosensor sensitivity and response profiles, overcoming key limitations inherent to single-site transcriptional reporter designs.

## References

[1] A. Vallée-Bélisle, F. Ricci, K. Plaxco, *J Am Chem Soc*, **2012**, *134*, 2876–2879.

**Erica Belforte<sup>1</sup>, Andrea Celeste Di Pede<sup>1</sup>, Alessandro Porchetta<sup>1</sup>**

<sup>1</sup> Department of Chemistry, University of Rome, Tor Vergata, Via della Ricerca Scientifica 00133, Rome, Italy

Email presenting author: erica.belforte@alumni.uniroma2.eu

### Text

DNA is constantly exposed to mutagenic agents that can damage its structure, posing significant health risks. Among the most common oxidative lesions is 8-oxo-7,8-dihydroguanine (8-oxoG), which often leads to G:C→T:A transversion mutations. When 8-oxoG pairs correctly with cytosine, the OGG1 glycosylase recognizes and removes it, initiating the BER pathway. If OGG1 fails to act, or if the lesion arises during replication, 8-oxoG can mispair with adenine, generating an 8-oxoG:A mismatch. This error is specifically recognized by the MUTYH glycosylase, which excises adenine to prevent mutagenesis. Mutations in the MUTYH gene cause MUTYH-associated polyposis (MAP), a hereditary cancer syndrome that markedly increases the risk of colorectal and other cancers. Current methods for assessing DNA repair activities are mostly indirect, often slow, with limited sensitivity and clinical applicability<sup>1</sup>. Only a few strategies enable direct monitoring of MUTYH activity, typically based on fluorescent DNA probes<sup>2</sup>, but these require complex synthesis and offer restricted sensitivity. Here we propose a synthetic biology toolkit for real-time analysis of MUTYH activity using programmable nucleic acids that convert glycosylase action into CRISPR-based ultrasensitive detection. The system relies on a rationally designed “DNA activator module,” a probe whose structural switch is controlled by glycosylase activity. Only in its ON state does the module activate Cas12a, producing a fluorescent signal.

### References

- [1] WILSON, David L.; KOOL, Eric T. Fluorescent probes of DNA repair. *ACS chemical biology*, 2017, 13.7: 1721-1733.
- [2] NAGEL, Zachary D., et al. Multiplexed DNA repair assays for multiple lesions and multiple doses via transcription inhibition and transcriptional mutagenesis. *Proceedings of the National Academy of Sciences*, 2014, 111.18: E1823-E1832.

# eXpanding CHEMistry: implementing excellence in research and teaching

## X-CHEM III year Meeting

December 18<sup>th</sup> Department of Chemical Science and Technologies

DNA condensates containing *client* silica nanoparticles (SiNPs) for theranostic applications

Laura Beltrán<sup>1</sup>, Emma Barilli<sup>2</sup>, Sofia Marzari<sup>2</sup>, Martina Persia<sup>1</sup>, Alessandro Bertucci<sup>2</sup>,  
Alessandro Porchetta<sup>1</sup>

<sup>1</sup>Dipartimento di Scienze e Tecnologie Chimiche, Università degli Studi di Roma "Tor Vergata", Via della Ricerca Scientifica 1, 00133-Rome, Italy

<sup>2</sup>Dipartimento di Scienze Chimiche, della Vita e della Sostenibilità Ambientale, Università degli Studi di Parma, Parco Area delle Scienze 17/A, 43124-Parma, Italy

Email presenting author: *laura.beltranchamorro@students.uniroma2.eu*

Biomolecular condensates – dynamic, biomolecule-enriched droplets which arise owing to Liquid-Liquid Phase Separation (LLPS) – have been recently described to be implicated in many key vital processes within cells [1,2]. Although intracellular LLPS is extremely complex, the use of nucleic acids' high programmability, governed by Watson–Crick–Franklin base-pairing, offers a straightforward mechanism to form predictable artificial condensates [2]. Specifically, DNA nanotechnology provides a powerful platform for the engineering of condensates with tuneable structures and functions [3,4].

Herein, we report on the partitioning of mesoporous silica nanoparticles (SiNPs) into DNA-based condensates. Our strategy leverages DNA nanostars which are rationally designed to include an anchoring single-stranded DNA (ssDNA) overhang for the recruitment of SiNPs functionalized with complementary DNA sequences. To explore the parameters governing nanoparticle partitioning, we constructed a toolbox of SiNPs varying in size (from 90 to 700 nm) and surface chemistry (DBCO-modified and carboxylated), allowing us to investigate the combined effects of particle size, surface properties, and sequence-specific hybridization on partitioning behaviour within the condensate. Our findings indicate that there is no strict size threshold limiting SiNP partitioning into DNA condensates and provide insights into how biomolecular condensates mediate selective client loading and molecular interactions.

## References

- [1] S. Brocca, R. Grandori, S. Longhi, V. Uversky. *Int. J. Mol. Sci.*, **2020**, *21*, 9045.
- [2] J. M. Stewart, S. Li, A. A. Tang, M. A. Klocke, M. V. Gobry, G. Fabrini, L. Di Michele, P. W. K. Rothemund, and E. Franco, *Nat. Commun.*, **2024**, *15*, 6244
- [3] S. Xu, Y. Ouyang, Y. Qin, D. Chen, Z. Duan, D. Song, D. Harries, F. Xia, I. Willner, and F. Huang, *Nat. Commun.*, **2025**, *16*, 3352
- [4] S. Zhou, X. Ju, H. Chen, Y. Zhang, J. Zheng, K. Wang, X. Yang, and J. Liu, *Angew. Chem. Int. Ed.*, **2025**, *64*, e202505316

# eXpanding CHEMistry: implementing excellence in research and teaching

## X-CHEM III year Meeting

December 18<sup>th</sup> Department of Chemical Science and Technologies

*Covalent Dynamic DNA Networks to Translate Multiple Inputs into Programmable Outputs*

*Simone Brannetti<sup>1</sup>, Serena Gentile<sup>2</sup>, Erica Del Grosso<sup>1</sup>, Sijbren Otto<sup>3</sup>, Francesco Ricci<sup>1</sup>*

<sup>1</sup> Department of Chemistry, University of Rome Tor Vergata, Via della Ricerca Scientifica, 00133 Rome, Italy;

<sup>2</sup> Catholic Universities sacred heart A. Gemelli 8 Rome;

<sup>3</sup> Centre for Systems Chemistry, Stratingh Institute, University of Groningen, Groningen, the Netherlands

Email presenting author: simone.brannetti@uniroma2.it

Many biochemical signal-processing pathways rely on families of proteins that competitively dimerize in diverse combinations. Such competitive dimerization networks enable complex input-output computations and context-specific adaptability by varying component expression levels.<sup>1</sup> Inspired by this biological occurring paradigm and introducing the predictability and sequence specificity of DNA hybridization, we propose the development of a synthetic DNA-based dimerization network capable of sophisticated computational ability.<sup>2</sup>

Our system employs DNA monomers functionalized with reactive groups that covalently bond to form dimer outputs in an all-to-all or many-to-many fashion. Inputs can selectively bind and sequester specific monomers, preventing them from participating in the dimerization process and thus controlling the network's outputs. This design enables highly programmable input-output computation, offering control over the synthesis of a selected dimer output. Furthermore, we demonstrate that the network's size and complexity can be readily scaled, significantly expanding its computational capacity. Notably, DNA-based dimerization networks can regulate the yield of functional dimers outputs to drive downstream reactions, such as the controlled assembly or disassembly of synthetic DNA nanostructures.<sup>3</sup> Building on these capabilities, we want to integrate enzyme-responsive modules, creating an additional regulatory layer that can dynamically control networks behavior.

## References

- [1] J. Parres-Gold, M. Levine, B. Emert, A. Stuart, M.B. Elowitz, "Contextual computation by competitive protein dimerization networks". *Cell.* **2025**, 188, 1984–2002.
- [2] J. Li; A. Green; H. Yan; C. Fan, *Nat. Chem.* **2017**, 9 (11), 1056–1067.
- [3] S. Brannetti, S. Gentile, E. Del Grosso, S. Otto, F. Ricci, *J. Am. Chem. Soc.* **2025**, 147, 7, 5755–5763.

# eXpanding CHEMistry: implementing excellence in research and teaching

## X-CHEM III year Meeting

December 18<sup>th</sup> Department of Chemical Science and Technologies

*Role of Interfacial Adhesion in the LF-MOD Growth of Epitaxial YBCO Films on LaAlO<sub>3</sub> and SrTiO<sub>3</sub>*

Michele De Angelis<sup>1,2</sup>, Michele Amato<sup>3</sup>, Alexandre Gloter<sup>3</sup>, Valentina Pinto<sup>2</sup>, Giuseppe Celentano<sup>2</sup>, Massimo Tomellini<sup>1</sup>

<sup>1</sup> Tor Vergata University, Dept. of Chemical Sciences and Technologies, Via della Ricerca Scientifica, 00133, Rome, Italy

<sup>2</sup> Superconductivity Laboratory, Dept. of Fusion and Technologies for Nuclear Safety and Security, ENEA, Via E. Fermi 45, 00044, Frascati (Rome), Italy

<sup>3</sup> Université Paris-Saclay, Lab. de Physique des Solides, 91405, Orsay (Paris), France

Email presenting author: [michele.deangelis.01@alumni.uniroma2.eu](mailto:michele.deangelis.01@alumni.uniroma2.eu)

The growth of epitaxial YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-Y</sub> (YBCO) films via chemical solution routes represents a promising path toward scalable, high-quality superconducting layers [1-7]. In particular, low-fluorine metal-organic decomposition (LF-MOD) has demonstrated the capability to yield high-performance YBCO films, minimizing fluoride content while preserving superconducting properties [4-6]. However, the final film quality appears to be critically dependent on interfacial adhesion and the atomic-scale stability at the precursor/substrate interface factors essential for controlled nucleation, epitaxial registry, and minimization of defects [5-7].

In this work, we emphasize the essential role of adhesion energy ( $W$ ) of the interface on the epitaxial growth of chemically derived YBCO thin films on single crystal perovskite substrates LaAlO<sub>3</sub> (LAO) and SrTiO<sub>3</sub> (STO). DFT calculations are used to compute interfacial energetics and adhesion energies for YBCO/LAO and YBCO/STO systems, demonstrating a more favorable interfacial stability for YBCO on LAO than on STO. Complementary, high-resolution structural analyses (TEM and EELS) are proposed to experimentally determine the actual atomic terminations and crystallographic orientation of YBCO on both substrates, enabling a direct correlation between theoretical predictions and real interfacial structure. This combined theoretical-experimental approach aims to provide a robust framework for optimizing LF-MOD growth processes of YBCO on commercial substrates.

## References

- [1] X. Obradors et al, *Supercond. Sci. Technol.*, **2012**, *25*, 123001.
- [2] X. Obradors et al, *Physica C: Superconductivity and its Applications*, **2012**, *482*, 58.
- [3] V. F. Solovyov et al, *Supercond. Sci. Technol.*, **2005**, *18*, 239.
- [4] V. Pinto et al, *IEEE Trans. Appl. Supercond.*, **2018**, *28*, 7500505.
- [5] V. Pinto et al, *Supercond. Sci. Technol.*, **2020**, *33*, 115006.
- [6] M. De Angelis and M. Tomellini, *J. of Physics D: Applied Physics*, **2024**, *57*, 465301.
- [7] M. De Angelis et al, *J. of Physics D: Applied Physics*, **2025**, *58*, 115302.

# eXpanding CHEMistry: implementing excellence in research and teaching

## X-CHEM III year Meeting

December 18<sup>th</sup> Department of Chemical Science and Technologies

*Silica nanohelices coated with porphyrins as hybrid materials for detecting volatile enantiomers*

Iulia Di Filippo<sup>1</sup>, Zakaria Anfar<sup>2</sup>, Reiko Oda<sup>2</sup>, Gabriele Magna<sup>1</sup>, Donato Monti<sup>3</sup>, Corrado Di Natale<sup>4</sup>, Roberto Paolesse<sup>1</sup>, Manuela Stefanelli<sup>1</sup>

<sup>1</sup>Department of Chemical Science and Technologies University of Rome Tor Vergata, Rome, Italy

<sup>2</sup>University of Bordeaux, CNRS, Bordeaux INP, CBMN, UMR 5248, 33600 Pessac France

<sup>3</sup>Department of Chemistry, University of Rome La Sapienza, Rome, Italy,

<sup>4</sup>Department of Electronic Engineering, University of Rome Tor Vergata, Rome, Italy

Email presenting author: [ilaria.di.filippo@uniroma2.it](mailto:ilaria.di.filippo@uniroma2.it)

Chiral recognition is a key challenge in diverse fields, including agrochemicals, environmental science, and health monitoring. In this study, we applied the electronic nose (e-nose) approach for chiral recognition by employing hybrid chiral materials composed of silica nanohelices covalently functionalized with chiral porphyrins ((D)/(L)-ZnP) and an achiral porphyrin (ZnPCTTP). The materials were characterized using FTIR, UV-Vis, and CD spectroscopies and TEM microscopy. The Circular Dichroism (CD) spectroscopy demonstrated that the overall chirality is mainly related to helices handedness. The suspensions of the materials were deposited on Quartz Microbalance (QMB) surfaces to create an e-nose array consisting of six chiral sensors and an achiral one, used as a reference. This array was tested toward vapors of five pairs of pure enantiomers at various concentrations. Linear Discriminant Analysis (LDA) was employed to assess the classification performance in two scenarios: an "achiral" task with 5 classes where enantiomers were grouped together, and a chiral recognition task with 10 classes where each enantiomer was treated as a distinct class. The results demonstrated almost perfect performance in identifying both the compounds and their enantiomers [1].

## References

[1] I. Di Filippo, Z. Anfar, G. Magna, P. Pranee, D. Monti, M. Stefanelli, R. Oda, C. Di Natale, R. Paolesse *Nanoscale Adv.* **2024**, *122*, 27, 6.

# eXpanding CHEMistry: implementing excellence in research and teaching

## X-CHEM III year Meeting

December 18<sup>th</sup> Department of Chemical Science and Technologies

*Triplex DNA Clamp Regulates Cas12a Activation for ssDNA and RNA Sensing*

*Andrea Celeste Di Pede<sup>1</sup>, Neda Bagheri<sup>1</sup>, Erica Belforte<sup>1</sup>, Alessio Palone<sup>1</sup>, Marianna Rossetti<sup>1</sup> and Alessandro Porchetta<sup>1</sup>*

<sup>1</sup> Department of Chemical Sciences and Technologies, University of Rome, Tor Vergata, Via della Ricerca Scientifica 00133, Rome, Italy

Email presenting author: Andrea.Celeste.Di.Pede@uniroma2.it

## Text

The widespread use of CRISPR in diagnostics stems from the discovery that Cas12 and Cas13 exhibit collateral, non-specific cleavage upon binding DNA or RNA targets. [1] Cas12, an RNA-guided nuclease, can recognize both single- and double-stranded DNA and simultaneously amplify signals through this collateral activity, which is commonly exploited using fluorophore–quencher DNA probes. [2] In this work, we present a molecular strategy that enables programmable activation of the CRISPR-Cas12a system in response to triplex DNA formation triggered by single-stranded DNA (ssDNA) or RNA inputs. Our triplex-controlled Cas12a assay leverages the high specificity of clamp-like triplex structures to control a toehold-based strand displacement reaction within a rationally designed DNA hairpin (PAM-Switch). Upon displacement and PAM complementation, the Cas12a ribonucleoprotein (RNP) is activated, initiating trans-cleavage and producing a concentration-dependent fluorescent signal. By separating target recognition (via triplex formation) from direct Cas12a–crRNA binding, the assay removes the need for target-specific crRNAs and enables multiple target detection within a single reaction mix. The use of triplex-based clamps provides high specificity for single-nucleotide variants and allows sensitive detection of ssDNA and RNA targets 10–20 nt long, overcoming key limitations of current Cas12 diagnostics.

## References

- [1] L. Shi-Yuan, C. Qiu-Xiang, W. Jing-Man, L. Xiao-Yan, Z. Zi-Long, G. Song, C. Rui-Bing, Z. Guo-Ping, and W. Jin, *Cell Discov* 4, 20 (2018).
- [2] M. Rossetti, R. Merlo, N. Bagheri, D. Moscone, A. Valenti, A. Saha, P. Arantes, R. Ippodrino, F. Ricci, I. Treglia, E. Delibato, J. Van Der Oost, and A. Porchetta, *Nucleic Acids Research* 50 (2022) 8377 – 83961

# eXpanding CHEMistry: implementing excellence in research and teaching

## X-CHEM III year Meeting

### December 18<sup>th</sup> Department of Chemical Science and Technologies

*Hybrid Nanozyme System: Gold-Decorated Nanodiamonds for Electrochemical Sensing and SERS substrate*

*Beatrice Ercolani<sup>1</sup>, Antonio Licheri<sup>1</sup>, Valeria Gugliemotti<sup>1</sup>, Roberto Matassa<sup>2,3</sup>, Sara Tosi<sup>1</sup>, Silvia Orlanducci<sup>1</sup>*

<sup>1</sup>Department of Chemical Sciences and Technologies, University of Rome Tor Vergata, Via della Ricerca Scientifica 1, 00133, Rome, Italy

<sup>2</sup>Physics Division, School of Science and Technology, University of Camerino, 62032 Camerino, MC, Italy

<sup>3</sup> Department of Anatomical, Histological, Forensic and Orthopaedic Sciences, Section of Human Anatomy, Sapienza University of Rome, Via A. Borelli 50, 00161, Rome, Italy

[beatrice.ercolani@uniroma2.it](mailto:beatrice.ercolani@uniroma2.it)

## Abstract

Nanozymes are nanomaterials with enzyme-like catalytic activity and are increasingly used in sensing due to their high stability, reusability, low cost, and resistance to harsh conditions<sup>[1]</sup>. Gold nanoparticles (AuNPs) show excellent peroxidase-like activity, making them attractive for sensing applications<sup>[2][3]</sup>. However, conventional AuNP synthesis methods often require reducing and stabilizing agents that can reduce catalytic efficiency, motivating the development of alternative strategies<sup>[4]</sup>.

In this work, gold-decorated nanodiamonds (AuNP-NDs) are proposed as a novel hybrid platform for electrochemical sensors and surface-enhanced Raman spectroscopy (SERS). The AuNP-ND system exhibits enhanced catalytic performance, confirmed by UV-vis analysis, and a significant SERS response. The hybrid material combines strong peroxidase-like activity with improved operational stability. For electrochemical applications, AuNP-NDs were deposited onto graphite working electrodes of screen-printed electrodes on PET substrates. Probe-free electrochemical detection was carried out by continuous chronoamperometry for hydrogen peroxide sensing, confirming the suitability of the material for the quantitative determination of H<sub>2</sub>O<sub>2</sub>. In addition, probe-free SERS detection of hydrogen peroxide was performed, allowing its direct identification without molecular reporters and clearly confirming the SERS activity of the hybrid material for sensing applications.

## References

- [1] M. Zandieh, J. Liu, *Advanced Materials* **2024**, 36, 2211041.
- [2] J. Lou-Franco, B. Das, C. Elliott, C. Cao, *Nanomicro Lett* **2021**, 13.
- [3] Y. Mikami, A. Dhakshinamoorthy, M. Alvaro, H. García, *Catal Sci Technol* **2013**, 3, 58.
- [4] I. Hammami, N. M. Alabdallah, A. Al jomaa, M. kamoun, *J King Saud Univ Sci* **2021**, 33, 101560.

*Synthesis and Characterization of Photocurable, Smart and Semi-interpenetrated Hydrogels*

*Ozge Eslek<sup>1</sup>, Fabio Domenici<sup>1</sup>, Gaio Paradossi<sup>1</sup>*

<sup>1</sup> Department of Chemical Science and Technologies, University of Rome Tor Vergata,

Via della Ricerca Scientifica 00133, Rome, Italy

ozge.eslek@uniroma2.it

Poly(vinyl alcohol) (PVA) is a synthetic, water-soluble, and biocompatible polymer suitable for a wide range of applications, particularly in the biomedical field. PVA-based hydrogels, which consist of cross-linked three-dimensional polymer networks, exhibit a strong capacity for water absorption and possess good mechanical properties. These features enable their use in different applications, including drug delivery, wound dressings, self-healing materials, and tissue engineering [1]. Smart hydrogels are capable of responding to external stimuli, such as temperature, magnetic fields, and pH, and return to their initial state once the stimulus is terminated [2]. More specifically, Poly(N-isopropylacrylamide) (p(NipAAm))-based hydrogels undergo thermal transition near physiological temperature, making them highly attractive for drug delivery and other biomedical applications [3]. Collagen is the most abundant protein in animals and a crucial component of the extracellular matrix (ECM), a complex structural network that anchors neighboring cells, provides mechanical support to tissues and organs, and regulates cellular activities [4]. Semi-interpenetrating (semi-IPN) networks are polymeric materials that are made of at least two types of polymer: one forms a cross-linked network, and the other (or others) is a linear or branched polymer physically entrapped within that network [5]. In this study, the PVA backbone was grafted with glycidyl methacrylate (GMA) to obtain photocurable hydrogels [6, 7]. Furthermore, we obtained a smart polymeric network through the copolymerization of N-isopropylacrylamide (NipAAm) monomer into the PVA-MA backbone [8, 9]. The thermo-responsivity at  $35.2 \pm 0.5$  °C was assessed by DSC and rheology. Finally, semi-IPN bioactive hydrogels were designed by entrapping collagen within the network, and their protein-release profile as well as their mechanical properties were evaluated.

**References**

- [1] F. Carton, et al., *Int. J. Mol. Sci.*, **2024**, *25*, 11426.
- [2] S. Jahanbekam, et al., *J. Drug Deliv. Sci. Technol.*, **2025**, *107*, 106758.
- [3] E. S. Gil and S. M. Hudson, *Progress in Polymer Science*, **2004**, *29*, 1173-1222.
- [4] Shoulders M.D., Raines RT, *Annu Rev Biochem.* **2009**, 78:929-958.
- [5] C. D. Varganic, et al., *Materials & Design*, **2021**, *212*, 110237.
- [6] G. Paradossi et al., *Journal of Materials Science: Materials in Medicine*, **2003**, *14*, 687-91.
- [7] F. Cavalieri, F. Miano, P. D'Antona, and G. Paradossi, *Biomacromolecules*, **2004**, *5*, 2439-46.
- [8] S. V. Ghugare, et al., *Macromolecules*, **2011**, *44*, 4470-78.
- [9] S. V. Ghugare et al., *J Phys Chem B*, **2010**, *114*, 10285-93.

# eXpanding CHEMistry: implementing excellence in research and teaching

## X-CHEM III year Meeting

December 18<sup>th</sup> Department of Chemical Science and Technologies

*Synthesis of Iron-N-methyl corroles as chiral catalysts*

Alessia Fata<sup>1</sup>, Francesco Pizzoli<sup>1</sup>, Roberto Paolesse<sup>1</sup>, Sara Nardis<sup>1</sup>

<sup>1</sup>University of Rome Tor Vergata, Via della Ricerca Scientifica 1, 00133 Rome, Italy

Email presenting author: alessia.fata@students.uniroma2.eu

Corroles represent a versatile group of compounds that exhibit remarkable coordination flexibility, enabling the incorporation of various metals.[1] Their distinctive reactivity and photophysical properties enable their application as sensing materials in chemical sensors for optical, electrochemical, and conductometric transducers.[2] The catalytic activity has also been investigated and reported in several publications; iron corroles are more selective catalysts than porphyrin analogues for the aziridination of olefins,[3] and specific functionalizations on their meso positions can be explored for applications in electrocatalysis.[4] Furthermore, the use of metallocorroles resulted in a very powerful cooperative catalytic system for CO<sub>2</sub> fixation with epoxides.[5] In this work, we studied the catalytic activity of meso-arylcorrole complexes and their N-methyl analogues. We used the N-substituted macrocycles to introduce an interesting dimension, considering their relatively unexplored chirality in catalysis. We aim to investigate their performance in two types of catalytic strategies for the synthesis of chiral fine chemicals, starting from prochiral compounds: CO<sub>2</sub> insertion reactions with aziridines, for oxazolidinones synthesis, and the insertion of diazo compounds, into N-H bonds of amines for amino ester synthesis, could provide valuable insights into their potential as enantioselective catalysts and contribute to the development of greener synthetic methodologies.

## References

- [1] S. Nardis, F. Mandoj, M. Stefanelli, R. Paolesse, *Coord. Chem. Rev.*, **2019**, *388*, 360–405.
- [2] R. Paolesse, S. Nardis, D. Monti, M. Stefanelli, C. Di Natale, *Chem. Rev.*, **2017**, *117*, 2517–2583.
- [3] L. Simkhovich, Z. Gross, *Tetrahedron Lett.*, **2001**, *42*, 8089–8092.
- [4] W. Sinha, A. Mahammed, N. Fridman, Z. Gross, *ACS Catal.*, **2020**, *10*, 3764–3772.
- [5] M. Tiffner, S. Gonglach, M. Haas, W. Schöfberger, M. Waser, *Chem. Asian J.*, **2017**, *12*, 1048–1051.

## Phase-change heterostructures based on MoSe<sub>2</sub> intercalated with Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub>

A. Foglietti<sup>1,2</sup>, S. De Simone<sup>1\*</sup>, S. Calvi<sup>1,3</sup>, A. Díaz Fattorini<sup>1,3</sup>, C. Petrucci<sup>1,3</sup>, F. Arciprete<sup>1,3</sup>,  
R. Calarco<sup>1</sup> and M. Longo<sup>2,1</sup>

<sup>1</sup>Institute for Microelectronics and Microsystems (IMM), Consiglio Nazionale delle Ricerche (CNR), Via del Fosso del Cavaliere 100, 00133 Rome, Italy;

<sup>2</sup> Department of Chemical Science and Technologies, University of Rome Tor Vergata, Via della Ricerca Scientifica 1, 00133 Rome, Italy;

<sup>3</sup> Department of Physics, University of “Tor Vergata”, Via della Ricerca Scientifica 1, 00133 Rome, Italy.

Email presenting author: agnese.foglietti@students.uniroma2.eu

### Text

The development of Ge-Sb-Te phase change materials is of growing interest for non-volatile memory devices, as they allow a fast and reversible switch from the amorphous and crystalline phases, involving a resistivity contrast for digital encoding. Both the integration of transition metal dichalcogenides [1] and the use of multilayer chalcogenide architectures [2] have been shown to improve the thermal stability, influence crystallization dynamics, and enable enhanced functionality in phase-change memory devices. To explore these advantages, in this work thin films of MoSe<sub>2</sub> were grown by RF-sputtering at room temperature and integrated into MoSe<sub>2</sub>/Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> (GST225) phase-change heterostructures to evaluate their effectiveness as confinement layers for heat and interdiffusion. The structural and morphological properties of the films were examined using temperature-dependent X-Ray Diffraction (XRD), Atomic Force Microscopy and Scanning Electron Microscopy. The grown MoSe<sub>2</sub> single-layers exhibited a uniform morphology at the nanoscale, and their crystallization was observed between 250 °C and 300 °C. Multilayers composed of alternating GST225 and thin MoSe<sub>2</sub> layers were then fabricated and annealed. The diffraction peaks in the XRD patterns showed no shift, indicating that MoSe<sub>2</sub> and GST225 maintain their structural integrity without intermixing. These results demonstrate the structural stability of sputtered MoSe<sub>2</sub> and highlight the potential of MoSe<sub>2</sub>/GST225 heterostructures for advanced phase-change memory devices.

### References

1. K. Ding, et al., *Science*, 2019, 366, 210–215
2. B. M., et al., *Sci. Rep.*, 2024, 14, 15713

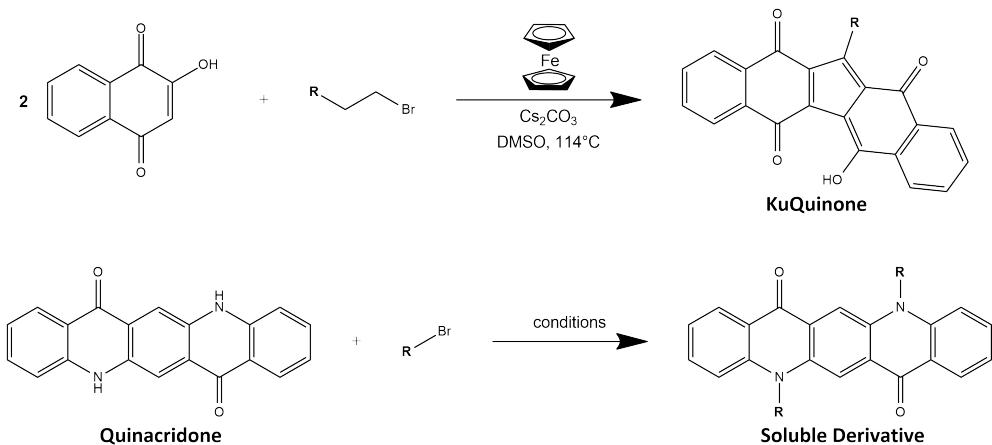
*Synthesis of Novel Organic Dyes for Light Driven Applications*

*Alessandro Iannini<sup>1</sup>, Veronica Spinelli<sup>1</sup>, Maria G. Iaquaniello<sup>1</sup>, Lorenzo Tommasi<sup>1</sup>, Valeria Conte<sup>1</sup>, Federica Sabuzi<sup>1</sup> and Pierluca Galloni<sup>1</sup>.*

<sup>1</sup> Department of Chemical Science and Technologies, University of Rome Tor Vergata, Via della Ricerca Scientifica, Rome, 00133.

Email presenting author: [alessandro.iannini@uniroma2.it](mailto:alessandro.iannini@uniroma2.it)

KuQuinones have recently emerged as a structurally distinctive and remarkable sub class of quinones. These compounds exhibit noteworthy electrochemical and absorption features, which reflect their sensitivity to the chemical environment. Their excellent photostability, combined with a high excited-state reduction potential (+2.12 to +2.16 V vs.NHE), makes them particularly appealing for light-driven oxidative processes<sup>1</sup>. Quinacridone's limited solubility has restricted its use in functional applications. Structural modifications have enabled the development of soluble derivatives with enhanced optical and electronic features. These dyes display broad visible absorption and a bimodal redox profile, making them promising for light-driven transformations<sup>2</sup>. In this work, the synthesis of new KuQs as well as QA derivatives has been pursued. Photo(electro)-chemical studies were also carried out to assess the performance of selected KuQs as photoanodes.



**Scheme 1** General Synthesis of KuQ and QA derivatives

**References**

- [1] F. Valentini, F. Sabuzi, M. Forchetta, V. Conte, P. Galloni, *RSC Adv.*, **2023**, *13*, 9065.
- [2] M. Forchetta, V. Baia, F. Sabuzi, V. Conte, P. Galloni, *Eur. J. Org. Chem.*, **2023**, *26*, e202300523.

# eXpanding CHEMistry: implementing excellence in research and teaching

## X-CHEM III year Meeting

December 18<sup>th</sup> Department of Chemical Science and Technologies

Programming transcription delay in cell-free systems

Jordy Alexis Lerma-Escalera<sup>1</sup>, Juliette Bucci<sup>1,2</sup>, Ana Urošević<sup>1</sup>, Romain Amador<sup>1</sup>,  
Gianfranco Ercolani<sup>1</sup> and Francesco Ricci<sup>1</sup>

<sup>1</sup>Department of Chemical Sciences and Technologies, University of Rome Tor Vergata,  
Rome, Italy.

<sup>2</sup>Department of Chemical Engineering and Biotechnology, University of Cambridge, Philippa  
Fawcett Drive, Cambridge CB3 0AS, UK3.

Email presenting author: jordyalexis.10@gmail.com

### Text

*Cell-free transcription systems provide a versatile platform to study and implement genetic circuits<sup>1,2</sup>. Temporal regulation of gene expression in living systems has inspired synthetic circuits with similar dynamics, yet their architectures are often complex and hard to tune<sup>3-6</sup>. We report here the design of orthogonal, enzyme-driven DNA transcriptional timers that enable precise programming of time delays in cell-free in vitro transcription. These timers utilize blocker strands that transiently bind to the promoter domain, preventing transcription onset. Selective enzymatic cleavage of the blocker strands triggers their removal, allowing input DNA strands to bind and initiate transcription. By tuning the kinetics of enzymatic blocker degradation - through varying enzyme or blocker strand concentrations - we achieve fine temporal control over transcription half-life ( $t_{1/2}$ ) from  $0.48 \pm 0.02$  h up to  $8.4 \pm 0.1$  h. Using three different blocker-degrading enzymes (RNase H, UDG, Fpg) we also demonstrate orthogonal temporal control of multiple transcription templates in a single solution. Finally, we show the programmed termination control and downstream regulation of Cas12a enzymatic collateral cleavage activity through such transcription timers. Together, these orthogonal DNA transcriptional timers establish a generalizable and straightforward framework for programming time-resolved transcription and gene expression in cell-free synthetic biology.*

### References

- [1] N. E. Gregorio, M. Z. Levine, J. P. Oza, Methods Protoc., 2019, 2, 24.
- [2] T. Wang, Y. Lu, Biosensors (Basel), 2022, 12, 318.
- [3] X. Li, Q. Qi, Q. Liang, Biotechnol. Biofuels Bioprod., 2023, 16, 158.
- [4] D. Pinto, et al., Nucleic Acids Res., 2018, 46, 7450–7464.
- [5] R. Maithreye, R. R. Sarkar, V. K. Parnaik, S. Sinha, PLoS One, 2008, 3, e2972.
- [6] W. Weber, et al., Proc. Natl. Acad. Sci. USA, 2007, 104, 2643–2648.

# eXpanding CHEMistry: implementing excellence in research and teaching

## X-CHEM III year Meeting

### December 18<sup>th</sup> Department of Chemical Science and Technologies

*Click Chemistry-Mediated Attachment of Spacers on Biochar: A Smart Tool for Robust and Reproducible Biosensing*

Antonio Licheri<sup>1</sup>, Veronica Mattarelli<sup>1</sup>, Claudia Mazzuca<sup>1</sup>, Silvia Orlanducci<sup>1</sup>, Laura Micheli<sup>1</sup>,  
Riccardo Salvio<sup>1</sup>

<sup>1</sup> Department of Chemical Science and Technologies, Tor Vergata University of Rome, Via Della Ricerca Scientifica 1, 00133, Roma, Italy

Email presenting author: Antonio.Licheri@uniroma2.it

#### Text

Biochar, a carbon-rich material derived from biomass pyrolysis, is attracting interest for electrochemical sensors due to its low cost, good electrochemical performance and availability of functional groups for biomolecule immobilization<sup>1</sup>. However, its heterogeneous surface often causes random bioreceptor orientation, poor reproducibility and nonspecific fouling, limiting performance in complex matrices<sup>2</sup>.

Herein, we present a multistep chemical approach to introduce a flexible molecular spacer onto spent coffee ground-derived biochar via covalent attachment using azide–alkyne click chemistry. Each functionalization step was characterized by spectroscopic and electrochemical techniques, confirming successful modification. The resulting interface is stable and reproducible and provides improved spatial control of biorecognition elements, projecting them into the solution phase while reducing adsorption of large proteins<sup>3</sup>.

As a proof of concept, an alkaline phosphatase–based biosensor was evaluated using a model substrate. Compared to pristine biochar, the functionalized material exhibited enhanced analytical performance, showing a 38% increase in maximum catalytic current and a 2.3-fold increase in the apparent Michaelis–Menten constant, indicating improved enzyme accessibility and faster substrate turnover. Electrochemical impedance spectroscopy further confirmed antifouling behavior, with a 39% reduction in nonspecific adsorption.

#### References

- [1] Y. Zheng, C. Yu, L. Fu, *Green Anal. Chem.*, **2023**, 7, 100081.
- [2] D. Spanu, G. Binda, C. Dossi, D. Monticelli, *Microchim. J.*, **2020**, 159, 105506.
- [3] S. Gao, J. M. Guisan, J. Rocha-Martin, *Anal. Chim. Acta*, **2022**, 1189, 338907.

***MAIGRET: an antibody-responsive cell-free transcription system for CRISPR-based ultrasensitive immunoassay***

*Francesca Miceli<sup>1</sup>, Sara Bracaglia<sup>1</sup>, Daniela Sorrentino<sup>1,2</sup>, Alessandro Porchetta<sup>1</sup>, Simona Ranallo<sup>1</sup>, Francesco Ricci<sup>1</sup>*

<sup>1</sup> Department of Chemical Science and Technologies, University of Rome, Tor Vergata, Via della Ricerca Scientifica, 00133 Rome, Italy.

<sup>2</sup> Department of Mechanical and Aerospace Engineering and of Bioengineering, University of California at Los Angeles, 420 Westwood Plaza, Los Angeles, California 90095, United States.

Email presenting author: [francesca.cosimina.miceli@uniroma2.it](mailto:francesca.cosimina.miceli@uniroma2.it)

Here we report a two-step CRISPR-based immunoassay, named MAIGRET (Molecular Assay based on antibody-Induced Guide-RNA Enzymatic Transcription), which enables the sensitive and versatile detection of antibodies and other proteins by integrating the advantages of CRISPR based sensing with cell-free transcription systems.<sup>1</sup> The assay is based on the use of a responsive synthetic DNA template that trigger the cell-free *in vitro* transcription of a guide RNA strand only upon recognition of a specific target antibody. Such transcribed guide RNA is then used to activate the Cas12 enzyme, which can lead the cleavage of a fluorophore/quencher-labelled reporter and thus resulting in an increase in the measured fluorescence signal. MAIGRET achieves highly sensitive (detection limits in the low picomolar range), specific (no signal in the presence of non-target antibodies), and selective (effective even in complex samples) detection of target proteins. Thanks to its programmable design, the platform can be tailored for different targets, either in direct or competitive assay formats, and supports multiplexed detection using orthogonal CRISPR enzymes (e.g., Cas13), each coupled with a distinct, antibody-responsive transcriptional template. Considering the versatility of MAIGRET, we are currently developing an adaptation with a colorimetric readout by employing the collateral cleavage of a horseradish peroxidase (HRP)-DNA strand anchored on the magnetic beads as reporter system.

## References

[1] F. Miceli, S. Bracaglia, D. Sorrentino, A. Porchetta, S. Ranallo, F. Ricci, *Nucleic Acids Res.* **2025**, 53(6):gkaf238.

*Controlling in-vitro transcription through a DNA-based dimerization network*

Miriam Quattrociocchi<sup>1</sup>, Simone Brannetti<sup>1</sup>, Erica Del Grosso<sup>1</sup>, Francesco Ricci<sup>1</sup>

<sup>1</sup> Department of Chemical Sciences and Technologies, University of Rome “Tor Vergata”, Rome, Italy

Email presenting author: quattrociocchimiriam@gmail.com

### Text

Living systems offer multiple examples of how fundamental functions can emerge from the interaction of molecular networks. [1]. One such example is given by the competitive protein dimerization networks, in which monomers of proteins can interact to each other to form a wide library of possible output dimers. The upregulation of certain dimers can play a critical role in the activation of specific downstream biological pathways [2]. Our aim is to synthetically recreate those naturally occurring networks by using DNA as a material. In this work we build a competitive DNA dimerization network composed by DNA monomers functionalized with reactive groups that can covalently bonds to each other and create a combinatorial library of DNA dimer outputs [3]. By introducing specific DNA input that selectively sequester monomers, we can drive the formation of a desired DNA dimer, which activates a specific *in-vitro* transcription system. This method is highly versatile, allowing for precise modulation of transcriptional output by tuning the size of the network and the composition of input strands. Moreover, the programmability of the DNA-based dimerization networks facilitates orthogonal transcription of multiple fluorogenic aptamers by also using different enzymes. We were able to control complicated pathways and to mimic a sort of enzymatic cascade. These DNA networks provide a platform for performing complex input-output computations in a highly predictable and programmable manner.

### References

- [1] C. Sharma, A. Samanta, R. S. Schmidt, A. Walther. *J. Am. Chem. Soc.* 2023, 145 (32), 17819–17830
- [2] J. Parres-Gold, M. Levine, B. Emert, A. Stuart, M.B. Elowitz. *Cell.* 2025. doi: 10.1016/j.cell.2025.01.036.
- [3] S. Brannetti, S. Gentile, E. Del Grosso, S. Otto, F. Ricci. *J. Am. Chem. Soc.* 2025, 147, 7, 5755–5763.

# eXpanding CHEMistry: implementing excellence in research and teaching

## X-CHEM III year Meeting

December 18<sup>th</sup> Department of Chemical Science and Technologies

### *Harnessing Nanodiamond Films for Photon-Enhanced Thermionic Emission*

*Raffaella Salerno<sup>1,2</sup>, Alessandro Bellucci<sup>2</sup>, Eleonora Bolli<sup>2</sup>, Matteo Mastellone<sup>2</sup>,  
Veronica Valentini<sup>2</sup>, Riccardo Polini<sup>1</sup> and Daniele Maria Trucchi<sup>2</sup>*

<sup>1</sup> Dipartimento di Scienze e Tecnologie Chimiche, Università di Roma “Tor Vergata”, 00133 Roma, Italy

<sup>2</sup> ISM-CNR, DiaTHEMA Lab, Via Salaria km 29.300, 00015 Monterotondo, Roma, Italy

Email presenting author: eleonora.bolli@cnr.it

Photon-Enhanced Thermionic Emission (PETE)<sup>1</sup> has emerged as a promising mechanism for concentrated solar energy conversion due to its ability to efficiently utilize both photon energy and thermal energy, thereby overcoming the limitations of traditional photovoltaic and thermionic devices. Our work explores the role of nanostructured silicon-diamond structures<sup>2</sup> as cathodes in PETE converters.

We employed microwave plasma-assisted chemical vapor deposition (MWPA-CVD) to grow diamond films on silicon wafers, examining both intrinsic and nitrogen-doped diamond. Initially, we conducted a study of the evolution and etching of detonation nanodiamond (DND) seeds to optimize the MWPA-CVD parameters for diamond growth<sup>3</sup>. The temporal evolution of DND seeds during the initial diamond growth phase was analyzed to maintain sufficient seed density, thereby achieving continuous diamond films as thin as 40 nm<sup>4</sup>.

Diamond layer optimization was achieved by assessing the influence of film thickness and comparing the properties of intrinsic versus nitrogen-doped diamond. The introduction of nitrogen doping enhanced electron emission, possibly due to the improvement in band alignment between silicon and diamond.

Femtosecond laser nanostructuring was applied to the silicon surface, to improve light management, creating uniform nanostructures and resulting in a tenfold increase in current density of the overall photocathode under concentrated solar illumination.

## References

- [1] J. W. Schwede, I. Bargatin, D. C. Riley, B. E. Hardin, S. J. Rosenthal, Y. Sun, F. Schmitt, P. Pianetta, R. T. Howe, Z.-X. Shen, N. A. Melosh, *Nat. Mater.*, **2010**, *9*, 762–767.
- [2] T. Sun, F. A. M. Koeck, A. Rezikyan, M. M. J. Treacy, R. J. Nemanich, *Phys. Rev. B*, **2014**, *90*, 121302-121307.
- [3] R. Salerno, B. Pede, M. Mastellone, V. Serpente, V. Valentini, A. Bellucci, D. M. Trucchi, F. Domenici, M. Tomellini, R. Polini, *ACS Omega*, **2023**, *8*, 25496–25505.
- [4] R. Salerno, V. Valentini, E. Bolli, M. Mastellone, V. Serpente, A. Mezzi, L. Tortora, E. Colantoni, A. Bellucci, R. Polini, D. M. Trucchi, *ACS Appl. Energy Mater.*, **2024**, *7*, 868–873.

# eXpanding CHEMistry: implementing excellence in research and teaching

## X-CHEM III year Meeting

### December 18<sup>th</sup> Department of Chemical Science and Technologies

#### Immune-induced antibody-DNA hybrid condensates

*Sara Scalia<sup>1</sup>, Marco Cappa<sup>2</sup>, Lorenzo Rovigatti<sup>2</sup>, Erica Del Grosso<sup>1</sup>, Francesco Ricci<sup>1</sup>*

<sup>1</sup>Department of Chemical Sciences and Technologies, University of Rome, Tor Vergata, Rome, Italy

<sup>2</sup>Department of Physics, University of Rome, Sapienza, Rome, Italy

Email presenting author: [sara.scalia@uniroma2.it](mailto:sara.scalia@uniroma2.it)

DNA condensates have garnered increasing interest as synthetic analogs of living cells or membraneless compartments, offering potential applications in various fields [1]. While membraneless organelles in cells typically form through complex protein–protein or protein–nucleic acid interactions [2], synthetic DNA condensates are generally formed by specific DNA–DNA interactions [3] or non-specific interactions [4]. To mimic the diversity of biomolecular interactions involved in the cellular microenvironment, we present here the combined use of specific DNA–DNA and antibody–antigen interactions to induce the formation of antibody–DNA hybrid condensates. To do this, we modified a four-arm DNA nanostar by replacing one sticky-end with one antigen. Only in the presence of the specific bivalent antibody, such nanostars phase-separate to form hybrid condensates. To demonstrate the versatility of the system, we employed multiple antigen-conjugated nanostars and their respective antibodies, achieving orthogonal and specific molecular recognition. The antibody–DNA hybrid condensates are also reversible and can be cyclically formed/dissolved by the cyclic degradation/addition of the specific antibody. This system might be used as an approach for applications in sensing and drug delivery.

## References

- [1] G. R. Abraham, A. S. Chaderjian, A. B. N Nguyen, S. Wilken, O. A. Saleh, *Rep. Prog. Phys.* **2024**, 87 (6), 066601.
- [2] S. F. Banani, H. O. Lee, A. A. Hyman, M. K. Rosen, *Nat. Rev. Mol. Cell Biol.* **2017**, 18, 285–98.
- [3] S. Biffi, R. Cerbino, F. Bomboi, E. M. Paraboschi, R. Asselta, F. Sciortino, T. Bellini, *Proc. Natl. Acad. Sci. U.S.A.* **2013**, 110 (39), 15633–37.
- [4] R. Merindol, S. Loescher, A. Samanta, A. Walther, *Nat. Nanotechnol.* **2018**, 13, 730–38.

## Dottorato **Materials for Sustainable Development**

1. Ni-Doping Strategies for Composite Fuel Electrodes of Solid Oxide Fuel Cells

Michela Cornale

2. Dense electrolytes fabrication and innovative deposition technique for integration in ProtonConducting Fuel Cells

Lorenzo Freschi

3. One-Pot Synthesis of LaNiO<sub>3</sub> for Enhanced Oxygen Evolution Reaction Activity in Alkaline Media

Pagano Giorgio

4. Ir-modified NiFe alloys for the Oxygen Evolution Reaction Electrocatalysis in Acidic and Alkaline media

Manuela Montalto

5. Functionalized materials with Essential Oils for Ecofriendly Antimicrobial Nanocoatings

Elisa Recchia

6. Controlled Microfluidic Synthesis of Cerium Oxide Nanoparticles

Beatrice Bruno

7. Theoretical and experimental analysis of solar fuels production processes coupled with CSP technology

Matteo Battaglia

8. Evaluating Force-Field Refinements in RNA Molecular Dynamics: A Comparative Analysis of OL3 and CMAP Corrections in the HuR–Aptamer Complex

Fabio Giovanni Tucci

9. Point-of-care diagnosis of orthopedic infections through a scalable and highly-sensitive printed pH sensor based on Carbon Black/Polyaniline nanocomposite

Christian Gosti

10. Preliminary characterization of a novel ruthenium dye-helical peptide conjugated system for DSSC enhanced performance

Valerio Cuboni

11. Targeting HuR: Exploring RNA Aptamers as a Novel Therapeutic Strategy

Davide Pietrafesa

12. Optimization of Self-Healing and Anticorrosive Properties of Waterborne Polyurethane Coatings for the Protection of Metallic Artworks

Elodia Spinelli

13. Integrating paper-based (bio)sensors in a novel Origami Organ-on-a-Chip Device: PHOENIX-OoC

Laura Belcastro

*Theoretical and experimental analysis of solar fuels production processes coupled with CSP technology*

Battaglia M.<sup>1</sup>, Tizzoni A.C.<sup>2</sup>, Spadoni A.<sup>2</sup>, Corsaro N.<sup>2</sup>, Sau S.<sup>2</sup>, Roshan N.<sup>3</sup>, D'Ottavi C.<sup>1</sup>,  
Licoccia S.<sup>1,4</sup>

<sup>1</sup>Department of Chemical Science and Technologies, University of Rome TOR VERGATA

<sup>2</sup>ENEA TERIN-SSI-EAT

<sup>3</sup>University of Rome SAPIENZA

<sup>4</sup>Nast Center, University of Rome TOR VERGATA

Email presenting author: matteo.battaglia@uniroma2.it

## **Text**

Concentrated Solar Power (CSP) is one of the most promising green technologies for achieving net-zero targets by 2050. It can harness solar energy to generate electricity through thermal conversion cycles, produce high-temperature heat for industrial processes, and store large amounts of thermal energy that can be used in a variety of valuable applications.

Currently, one of the major challenges for the widespread adoption of CSP technologies is the concept of dispatchability, which refers to the ability to modulate electricity production based on demand. In this context, solar fuel generation, delivering high-quality energy in the form of electricity, has the advantage of solving the problem with temporal variations in supply as the final fuels are easy to store, and are compatible with the present transport sector. One of the most widely studied solar fuels is H<sub>2</sub>, viewed as an alternative source of energy for replacing fossil fuels especially where storage is essential. However, research is trying to investigate new alternatives that solve some H<sub>2</sub> characteristic issues, as storability and transportability.

Several methods have been investigated regarding H<sub>2</sub> production, studying thermochemical cycles and electrolytical processes. Also, a specific study of Sulfur is being carried out as alternative solar fuel, thanks to its good transportability compared to H<sub>2</sub>.

**eXpanding CHEMistry: implementing excellence in research and teaching**  
**X-CHEM III year Meeting, December 18<sup>th</sup> 2025**  
**Department of Chemical Science and Technologies**

*Integrating paper-based (bio)sensors in a novel Origami Organ-on-a-Chip Device:  
PHOENIX-OoC*

Laura Belcastro<sup>1</sup>, Luca Fiore<sup>2</sup>, Fabiana Arduini<sup>1</sup>

<sup>1</sup>Department of Chemical Science and Technologies, University of Rome Tor Vergata, Via della Ricerca Scientifica 1, Rome 00133, Italy

<sup>2</sup>SENSE4MED srl, via Bitonto 139, Rome 00133, Italy

Email presenting author: laura.belcastro@uniroma2.it

Organ-on-a-chip (OoC) technology has emerged as a powerful tool in biomedical research, offering clear advantages over traditional in vitro and in vivo models. These microfluidic systems aim to recreate key physiological and mechanical features of human organs and tissues, to provide physiologically relevant platforms for studying human biology, especially in drug treatment evaluation. [1] However, conventional OoCs can face challenges including air-bubble formation, limited real-time sensing, and complex fabrication. PHOENIX-OoC proposes a fully paper-based origami platform for OoC design, aiming at overcoming these limitations. Paper's flexibility, low cost, and unique fluidic properties enable cell co-cultures, integrated (bio)sensing, and controlled microfluidics. As a crucial monitoring element, PHOENIX-OoC aims to integrate in the device a paper-based electrochemical sensor array for continuous monitoring of relevant biomarkers, enabling real-time assessment of cells' status. Among them, sensors for pH, nitrate, and glucose were developed on wax-patterned paper, tailoring working electrodes with pH-sensitive film, nanomaterials, nitrate-selective membrane and glucose oxidase. The sensors were tested in standard solutions and yielded linear responses:  $y = (-0.048 \pm 0.002)x + (0.359 \pm 0.004)$  ( $R^2=0.981$ ) for nitrate;  $y = (-0.083 \pm 0.001)x + (0.763 \pm 0.007)$  ( $R^2=0.998$ ) for pH, and  $y = (-0.12 \pm 0.01)x - (0.7 \pm 0.1)$  ( $R^2=0.960$ ) for glucose. As OoC technologies advance, they are expected to transform drug development, reduce animal testing, and support personalized medicine.

## References

[1] B. Zhang and M. Radisic, *Lab Chip*, 2017, 17, 2395-2420.

## Acknowledgements

L. B. thanks PHOENIX-OoC project, funded under European Union's Horizon Europe EIC 2023 Pathfinder Open program, grant agreement No 101130395.

*Beatrice Bruno<sup>1,2</sup>, Emanuele Limiti<sup>2</sup>, Francesca Corsi<sup>1</sup>, Lina Ghibelli<sup>1</sup>, Alberto Rainer<sup>2</sup>, Enrico Traversa<sup>1</sup>*

<sup>1</sup>Università di Roma Tor Vergata, via della Ricerca Scientifica, 00133 Rome, Italy

<sup>2</sup>Università Campus Bio-Medico di Roma, via Alvaro del Portillo 21, 00128 Rome, Italy

Email presenting author: beatrice.bruno@uniroma2.it

In the 21st century, technological innovation and materials design are driven by the unique properties of nanostructured materials. Interest in nanoscience—due to its potential to improve human well-being—has intensified the focus on engineering advanced nanomaterials and on developing precise, scalable synthesis routes [1]. Traditional methods often show batch variability and limited scalability, whereas microfluidics offers improved control, reproducibility, and efficiency [2]. Cerium oxide nanoparticles are notable for redox activity, antioxidant behaviour, and biofilm inhibition. Acting as multifunctional nanozymes, they display both redox-dependent and redox-independent catalytic properties [3]. These features make them attractive for environmental, agricultural, and biomedical uses, including cancer therapy, antimicrobial treatments, biosurfactants, and biosensors [4].

This study presents a continuous-flow microfluidic method to synthesize cerium oxide nanoparticles starting from cerium nitrate and using N,N,N',N'-tetramethyl ethylenediamine and Pluronic F127 as a precipitating and templating agent, respectively. A custom chip with three inlets, a spiral channel, and a serpentine section was designed to improve control over reaction parameters and to enhance mixing. The resulting nanoparticles were thoroughly analysed by Dynamic Light Scattering, Transmission Electron Microscopy, and Scanning Electron Microscopy.

This work highlights microfluidics as a scalable and precise strategy for producing high-quality cerium oxide nanoparticles with increased product consistency.

## References

- [1] K. R. Makgwane, S. S. Ray, *J. Nanosci. Nanotechnol.*, **2014**, 14, 1338–1363.
- [2] L. Zhang, Q. Chen, Y. Ma, J. Sun, *ACS Appl. Bio Mater.*, **2020**, 3, 107–120.
- [3] F. Corsi, G. Deidda Tarquini, M. Urbani, I. Bejarano, E. Traversa, L. Ghibelli, *Nanomaterials*, **2023**, 13, 2803.
- [4] K. R. B. Singh, V. Nayak, T. Sarkar, R. P. Singh, *RSC Adv.*, **2020**, 10, 27194–27214.

***Ni-Doping Strategies for Composite Fuel Electrodes of Solid Oxide Fuel Cells***

Cornale Michela\*, Panunzi Anna Paola, Duranti Leonardo, Di Bartolomeo Elisabetta

Department of Chemical Science and Technologies, University of Rome Tor Vergata, Via della Ricerca Scientifica, 00133, Rome, Italy

Email: \* michela.cornale@uniroma2.it

Solid oxide fuel cells (SOFCs) are a well-established technology for energy storage and conversion. The current state-of-the-art fuel electrode materials are cermets based on nickel and yttria-stabilized zirconia (Ni-YSZ). However, these materials are prone to degradation due to coking, as well as nickel coarsening and agglomeration, particularly in carbon-rich environments. According to the literature, the primary strategy to mitigate these issues involves replacing Ni-YSZ cermets with nickel-doped fluorite and/or perovskite-structured materials as alternative fuel electrodes [1].

This study investigates two composite fuel electrodes. The first comprises an A-site-deficient perovskite,  $\text{La}_{0.4}\text{Ca}_{0.4}\text{TiO}_3$  (LCT), combined with Ni-doped gadolinium-doped ceria (NiGDC), a fluorite-structured material. The second consists of a Ni-doped perovskite titanate,  $\text{La}_{0.4}\text{Ca}_{0.4}\text{Ti}_{0.95}\text{Ni}_{0.05}\text{O}_3$  (LCTN), combined with GDC. Among perovskite oxides, titanates are favored due to their structural stability in reducing atmospheres [2]. A-site deficiency facilitates the formation of oxygen vacancies, thereby enhancing ionic conductivity. Ni doping improves electrocatalytic performance via exsolution [3]. An innovative synthetic approach is developed for LCT and LCTN, enabling a substantial reduction in the calcination temperature to 700°C, a significant decrease from the 1400°C reported in the literature [4].

Electrolyte-supported SOFC tests assess the fuel electrode performance of the developed materials.

## References

- [1] J. T. Irvine, D. Neagu, M. C. Verbraeken, C. Chatzichristodoulou, C. Graves, M. B. Mogensen, *Nature Energy*, **2016**, 1-13.
- [2] J. J. Alvarado Flores, M. L. Ávalos Rodríguez, G. Andrade Espinosa, J. V. Alcaraz Vera, *Int. J. Hydrog. Energy*, **2019**, 44, 12529-12542.
- [3] W. Fan, Z. Ren, Z. Sun, X. Yao, B. Yildiz, and J. Li, *ACS Energy Lett.*, **2022**, 7, 1223-1229.
- [4] G. Lee, J. H. Myung, A. B. Naden, O. S. Jeon, Y. G. Shul, J. T. S. Irvine, *Adv. Energy Mater.*, **2020**, 10, 1903693.

**Preliminary characterization of a novel ruthenium dye-helical peptide conjugated system for DSSC enhanced performance**

Valerio Cuboni,<sup>1</sup> Giulia Sarpi,<sup>1</sup> Gianmaria Belardi,<sup>1</sup> Raffaella Lettieri<sup>1</sup>, Mariano Venanzi,<sup>1</sup> Marta De Zotti,<sup>2</sup> Salvatore Genovese,<sup>3</sup> Fausto Puntoniero,<sup>3</sup> Luigi Vesce,<sup>1</sup> Emanuela Gatto<sup>1</sup>

<sup>1</sup>Università degli Studi di Roma Tor Vergata

<sup>2</sup>Università degli Studi di Padova

<sup>3</sup>Università degli Studi di Messina

*valerio.cuboni@uniroma2.it*

### Text

Dye-sensitized solar cells (DSSCs) are a promising alternative to silicon-based panels thanks to their low cost, simple fabrication, and good performance under low-light conditions. Among the photosensitizers used in DSSCs, ruthenium bipyridine complexes are widely studied for their high photochemical stability, broad absorption spectrum, and efficient electron transfer properties[1]. Helical peptides also play an important role in charge-transfer processes[2] due to their defined secondary structures and their ability to support mechanisms such as superexchange and hopping, making them attractive for improving DSSC efficiency and stability[3][4]. In our experimental work, we investigated the DSSC application of a new ruthenium bipyridine dye modified with a thymine unit on one bipyridine group, designed to exploit the natural hydrogen bonding between thymine and adenine to form a supramolecular SAM on a flat gold surface. The SAM consisted of three layers: a lipo-adenine and a helical peptide functionalized with thymine and adenine, enabling conjugation with  $[T\text{-Ru(bpy)}_3]^{2+}$ . The ruthenium complex was first characterized spectroscopically in solution to assess its photophysical behaviour. Subsequently, the film was assembled on a gold and FTO-TiO<sub>2</sub> electrode to examine photocurrent generation under different excitation wavelengths. Preliminary photocurrent responses confirm that the assembly was successfully achieved and reveal efficient interfacial charge transfer within the peptide-dye conjugated architecture.

### References

- [1] A. O. Adeloye et al. *Molecules* **2014**, *19*(8), 12421-12460
- [2] M. Kai et al. *J. Pept. Sci.* **2008**; *14*: 192–202
- [3] E. Gatto et al. *Energies* **2022**, *15*(15), 5632
- [4] E. Gatto et al. *Angew. Chem. Int. Ed.* **2019**, *58*(22), 7308

# eXpanding CHEMistry: implementing excellence in research and teaching

X-CHEM III year Meeting, December 18<sup>th</sup> 2025

Department of Chemical Science and Technologies

*Dense electrolytes fabrication and innovative deposition technique for integration in Proton-Conducting Fuel Cells*

*Freschi L.<sup>1,2</sup>, Novelli V.<sup>1</sup>, Della Seta L.<sup>1</sup>, Grilli M.L.<sup>1</sup>, Duranti L.<sup>2</sup>, Pumiglia D.<sup>1</sup>, Di Bartolomeo E.<sup>2</sup>*

<sup>1</sup> Energy Technologies and Renewable Sources Department, Italian National Agency for New Technologies, Energy and Sustainable Economic Development (ENEA), Casaccia Research Center, Via Anguillarese 301, 00123 Rome, Italy

<sup>2</sup> University of Rome Tor Vergata, Department of Chemical Science and Technologies, Via Della Ricerca Scientifica, 00133 Rome, Italy

Email presenting author: *lorenzo.freschi@students.uniroma2.eu*

## Text

Proton-Conducting Fuel Cells (PCFCs) offer a clean and efficient way to convert H<sub>2</sub> into electricity at intermediate temperatures (400-700 °C) overcoming limitations of high-temperature fuel cells (e.g. traditional SOFCs) and becoming a key technology within the H<sub>2</sub> value chain. In the PCFC manufacturing, the fabrication of homogeneous, crystalline, and dense electrolytes as well as cell components integration is still challenging. Several issues may be encountered (especially during high temperatures sintering processes) which are detrimental on electrolyte stability and conductivity [1]. Further efforts have to be made to develop manufacturing techniques that allow optimal electrolyte deposition and components integration. Pulsed Electron Deposition (PED) is an innovative technique for homogeneous thin film deposition with controlled thickness, while maintaining same target stoichiometry. Key advantages of PED, over other physical deposition techniques, include lower equipment cost and higher energy efficiency [2][3]. This PhD program aim to create the first PCFC manufacturing line in ENEA Casaccia from the synthesis of proton conducting electrolytes to the full cell integration. At first, the research focused on the production and characterization of Ba<sub>1,1</sub>Ce<sub>0,6</sub>Zr<sub>0,2</sub>M<sub>0,2</sub>O<sub>3-δ</sub> (M = Y, Gd) dense ceramic electrolytes by investigating different synthesis and sintering routes. Subsequently, PED technique was explored by carrying out first electrolyte deposition tests on commercial anodes.

## References

- [1] S. Guo, L. Jiang, Y. Li, P. Zhong, S. Adeeba Ismail, T. Norby, D. Han, *Adv. Funct. Mater.*, **2024**, 2304729
- [2] M. Nistor, N. B. Mandache, J. Perriere, *J. Phys. D: Appl. Phys.*, **2008**, 41, 165-205
- [3] A. Liguori, C. Gualandi, M. L. Focarete, F. Biscarini, M. Bianchi, *Coatings*, **2020**, 10-16

***Point-of-care diagnosis of orthopedic infections through a scalable and highly-sensitive printed pH sensor based on Carbon Black/Polyaniline nanocomposite***

Christian Gosti<sup>1</sup>, Luca Fiore<sup>1,2</sup>, Fabio Domenici<sup>1</sup>, Gennaro Gentile<sup>3</sup>, Silvano Del Gobbo<sup>4</sup>, Raffaele Vitiello<sup>5,6</sup>, Giulio Maccauro<sup>5,6</sup>, and Fabiana Arduini<sup>1,2</sup>

<sup>1</sup>Department of Chemical Science and Technologies, University of Rome “Tor Vergata”, via della Ricerca Scientifica, 00133 Rome, Italy.

<sup>2</sup>SENSE4MED, Via Bitonto 139, 00133 Rome, Italy.

<sup>3</sup>Institute for Polymers, Composites and Biomaterials, Italian National Research Council, via Campi Flegrei 34, 80078 Pozzuoli, Italy

<sup>4</sup>Italian National Agency for New Technologies, Energy and Sustainable Economic Development (ENEA), Via Anguillarese, 301, 00123, Rome, Italy.

<sup>5</sup>Università Cattolica del Sacro Cuore, Rome, Italy.

<sup>6</sup>Fondazione Policlinico Universitario Agostino Gemelli Istituto di Ricovero e Cura a Carattere Scientifico (IRCCS), Rome, Italy.

Email presenting author: christian.gosti@uniroma2.it

## Abstract

Orthopedic-related injuries are commonly managed through the implantation of medical devices during arthroplasty procedures. However, this surgical practice has a substantial impact on patient health, due to the significant risk of developing periprosthetic infections. Bacterial proliferation and metabolic activity on the surface of orthopedic implants induce a decrease in the pH of the surrounding synovial fluid, thereby making pH a valuable diagnostic indicator.<sup>1</sup> Several limiting factors, namely storage constraints and insufficient sensitivity, have prevented earlier potentiometric pH sensors from becoming scalable point-of-care diagnostic tools. To overcome these shortcomings, here we introduced an affordable potentiometric screen-printed pH electrode that integrates cost-effective Carbon Black (CB) nanomaterial with chemically stable, pH-responsive Polyaniline (PANI) to enable the detection of orthopedic infections. The CB/PANI nanocomposite dispersion was applied onto the working electrode via a simple drop-casting step, providing an easy and reliable method for sensor functionalization. Upon mixture optimization, the 90% CB – 10% PANI composite was selected due to its excellent dispersibility and its optimal balance of analytical features, including robust reproducibility, notable sensitivity, and reliable selectivity. The sensor also demonstrated prolonged long-term stability, when dry-stored at room temperature over one month. Lastly, validation in real synovial fluid samples revealed strong agreement with pH-meter readings and microbiological results.

## References

[1] I. Milošev, V. Levašič, J. Vidmar, S. Kovač, R. Trebše, Journal of Biomedical Materials Research Part B: Applied Biomaterials, 2017, 105 (8), 2507–2515.

## Acknowledgments

This work was supported by SENSE4MED project.

# eXpanding CHEMistry: implementing excellence in research and teaching

X-CHEM III year Meeting, December 18<sup>th</sup> 2025

Department of Chemical Science and Technologies

*Ir-modified NiFe alloys for the Oxygen Evolution Reaction Electrocatalysis in Acidic and Alkaline media*

M. Montalto<sup>1</sup>, \*, W. Freitas<sup>1</sup>, B. Mecheri<sup>1</sup>, A. D'Epifanio<sup>1</sup>

<sup>1</sup> Department of Chemical Science and Technology, University of Rome Tor Vergata, Rome, Italy.

\*manuela.montalto@uniroma2.it

## Text

Water electrolysis is a promising strategy for sustainable hydrogen production, yet its efficiency is hindered by the sluggish oxygen evolution reaction (OER).<sup>1</sup> Conventional noble metal catalysts (RuO<sub>2</sub>, IrO<sub>2</sub>) exhibit high activity but suffer from high costs, scarcity, and limited stability.<sup>2</sup> NiFe-based electrocatalysts have emerged as attractive alternatives due to their low cost and excellent activity, though their long-term stability remains a challenge.<sup>3</sup> In this work, we investigate the effect of the iridium (Ir) addition on the structural, morphological, and electrochemical properties of NiFe alloys. Structural (XRD) and morphological (SEM) analyses were performed, while electrochemical behavior was assessed through rotating disk electrode experiments in acidic (pH 1) and alkaline (pH 13) conditions using cyclic voltammetry (CV) and chronoamperometry (CA). The results provide preliminary information on the role of Ir incorporation in improving the stability and catalytic efficiency of NiFe-based materials for water splitting applications.

## References

- [1] M. Chatenet, B. Pollet, D. R. Dekel, F. Dionigi, J. Deseure, P. Millet, R. D. Braatz, M. Z. Bazant, M. Eikerling, I. Staffell, P. Balcombe, Y. Shao-Horn, H. Schäfer, *Chem Soc Rev*, **2022**, vol. 51, 4583
- [2] Y. Kang, Y. Guo, J. Zhao, B. Jiang, J. Guo, Y. Tang, H. Li, V. Malgras, M. A. Amin, H. Nara, Y. Sugahara, Y. Yamauchi, T. Asahi, *Small*, **2022**, vol. 18, 2203411
- [3] J. Zhao, J.J. Zhang, Z.Y. Li, X.H. Bu, *Small*, **2020**, vol. 16, 2003916

**One-Pot Synthesis of LaNiO<sub>3</sub> for Enhanced Oxygen Evolution Reaction Activity in Alkaline Media**

Pagano Giorgio<sup>1\*</sup>, Panunzi Anna Paola<sup>1</sup>, Duranti Leonardo<sup>1</sup>, Di Bartolomeo Elisabetta<sup>1</sup>

<sup>1</sup> Department of Chemical Science and Technologies, University of Rome Tor Vergata, Via della Ricerca Scientifica, 00133, Rome, Italy

Email presenting author: giorgio.pagano@uniroma2.it

Water electrolyzers powered by renewable energy offer an environmentally sustainable approach to hydrogen production [1]. The oxygen evolution reaction (OER) is the rate determining step of water electrolysis and expensive platinum group metal (PGM) oxides such as RuO<sub>2</sub> and IrO<sub>2</sub> are the state-of-the-art OER electrocatalysts [2]. In alkaline water electrolyzers [3], perovskite oxides such as LaNiO<sub>3</sub> have emerged as excellent PGM-free electrocatalysts thanks to their stability and high activity [4].

In this work, a one-pot solution combustion route is presented as a fast and practical method to enhance LaNiO<sub>3</sub> OER activity descriptors. The synthesis is based on a combination of low-cost fuels: glycine (Gly) and citric acid (CAM), which has not been previously explored for LaNiO<sub>3</sub> to the best of our knowledge. Compared to other wet-chemistry methods, the Gly + CAM synthesis yielded powders with superior textural properties, optimal Ni<sup>3+</sup>/Ni<sup>2+</sup> ratio and high intrinsic OER activity.

References:

- [1] Abdin, Z. *et al.* Hydrogen as an energy vector. *Renew. Sustain. Energy Rev.*, **2020**, 120, 109620.
- [2] Zhang, K. & Zou, R. Advanced Transition Metal-Based OER Electrocatalysts: Current Status, Opportunities, and Challenges, *Small*, **2021**, 17.
- [3] Chi, J. & Yu, H. Water electrolysis based on renewable energy for hydrogen production. *Chinese J. Catal.*, **2018**, 39, 390.
- [4] Falqueto, J. B., Hales, N., Schmidt, T. J. & Fabbri, E. Recent Advances in Nickel-Based Perovskite Oxides for the Electrocatalytic Oxygen Evolution Reaction in Alkaline Electrolytes. *ACS Mater Lett.*, **2024**, 6, 5227.

*Targeting HuR: Exploring RNA Aptamers as a Novel Therapeutic Strategy*

Davide Pietrafesa<sup>1,2</sup>, Alice Romeo<sup>1</sup>, Federico Iacobelli<sup>1</sup> and Mattia Falconi<sup>1</sup>

<sup>1</sup> Department of Biology, University of Rome “Tor Vergata”, 00133 Rome, Italy

<sup>2</sup> PhD program in Materials for Sustainable Development, Department of Chemical Sciences and Technology, University of Rome “Tor Vergata”, 00133 Rome, Italy

Email presenting author: davide.pietrafesa@uniroma2.it

## Text

RNA-binding proteins (RBPs) regulate post-transcriptional gene expression. HuR is a key RBP that stabilizes mRNAs by binding AU-rich elements (AREs) in 3'UTRs. It contains three RRM<sub>s</sub> (RRM1–3), but a full 3D structure is still unresolved. Using *in silico* approaches, our lab generated a full-length HuR–mRNA model.

Because HuR promotes tumor growth, it represents an important therapeutic target. Current small-molecule inhibitors lack specificity, whereas RNA aptamers offer high affinity and selectivity. König et al. (2007) identified five aptamer classes (A, B, C, D and orphan) that bind HuR RRM<sub>s</sub>, providing a basis for aptamer optimization.

Aptamer sequences from König et al. were modelled with AlphaFold3, and topology/coordinate files were prepared using AmberTools23. GaMD production runs were performed with AMBER23 (500-ns replicas), and trajectories were analysed with GROMACS 2024. The top five aptamers were also fragmented, recombined, modelled, and simulated using the same protocol.

RMSD analyses showed aptamer A4 to be the least stable, while A1, B1, B2 and D2 displayed the highest structural stability. PCA revealed restricted HuR conformational sampling when bound to A1, A2 and B2. MM/PBSA confirmed these results, identifying A1, A2, B2, B3 and D2 as the strongest binders.

High-affinity fragments for each RRM were combined to target RRM1–RRM2 and RRM3. MD simulations showed overall RMSD stability, with HuR-B3-A2 being the most stable complex. Experimental validation is ongoing.

## References

- [1] N. Ripin, et al., Proc. Natl. Acad. Sci., **2019**, 116, 2935–2944.
- [2] C.W. Schultz, et al., WIREs RNA, **2020**, 11, e1581.
- [3] J. König, et al., RNA, **2007**, 13, 614–622.
- [4] J. Abramson, J. Adler, J. Dunger, et al., Nature, **2024**, 630, 493–500.
- [5] R. Salomon-Ferrer, et al., WIREs Comput. Mol. Sci., **2013**, 3, 198–210.
- [6] J. Wang, et al., WIREs Comput. Mol. Sci., **2021**, e1521.
- [8] D.A. Case, et al., J. Comput. Chem., **2005**, 26, 1668–1688.
- [9] M.J. Abraham, et al., SoftwareX, **2015**, 1–2, 19–25.

## FUNCTIONALIZED MATERIALS WITH ESSENTIAL OILS FOR ECO-FRIENDLY ANTIMICROBIAL NANOCOATINGS

Elisa Recchia<sup>1</sup>, Luca Fiore<sup>2</sup>, Nathalie Totaro<sup>1</sup>, Amaia M. Goitandia<sup>3</sup>, Maialen Argaiz<sup>3</sup>, Miren Blanco<sup>3</sup>, Fabiana Arduini<sup>2</sup>, Florigio Lista<sup>1</sup>

<sup>1</sup>Defence Institute for Biomedical Sciences, Via Santo Stefano Rotondo, 4 - 00184 Rome, Italy

<sup>2</sup>Department of Chemical Science and Technologies, University of Rome Tor Vergata, Via Della Ricerca Scientifica 1, Rome, Italy

<sup>3</sup>Unidad de Química de superficies y Nanotecnología, Fundación Tekniker, Iñaki Goenaga 5 -20600 Eibar, Spain

Email presenting author: elisa.recchia@persociv.difesa.it

Antimicrobial-resistant bacterial infections are a serious threat to human health [1, 2].

The Horizon Europe RELIANCE project addresses this challenge by developing antimicrobial coatings based on mesoporous silica nanoparticles functionalized with metallic copper under controlled conditions of oxidation state and essential oils, going beyond the state of the art [3].

Within this project, we studied the antibacterial activity by testing eugenol, carvacrol, thymol, and menthol in solution against five bacterial strains (*E. coli*, *B. clausii*, *S. aureus*, *P. aeruginosa* and, *K. pneumoniae*) to select the best oil for nanoparticles functionalization. The Minimum Inhibitory Concentration, Minimum Bactericidal Concentration, and Time Killing Assay were evaluated for eugenol, carvacrol, thymol, and menthol against five bacterial strains. Thymol and carvacrol showed the greatest antibacterial activity. The killing assay confirmed the superior efficacy of these two oils by killing 99.9% of bacteria in 10' at lower concentrations than eugenol and menthol.

Considering also the virucidal results, nanoparticles were successfully synthetized and functionalized with copper hydroxide and carvacrol to impart broad-spectrum antimicrobial activity. These functionalized nanoparticles have obtained complete killing activity after 2 h of incubation on *E. coli*, and 95.1% against *S. aureus*.

The results highlighted the effectiveness of copper nanoparticles modified with carvacrol for application in antimicrobial coatings on high-touch surfaces.

### References

- [1] P.S. Stewart, J.W. Costerton, Antibiotic resistance of bacteria in biofilms, *Lancet*, **2001**, 14, 135-8.
- [2] World Health Organization. Global Action Plan on Antimicrobial resistance. Geneva, Switzerland: World Health Organization; **2015**.
- [3] B. Xu, S. Li, R. Shi, H. Liu, Multifunctional mesoporous silica nanoparticles for biomedical applications, *Signal Transduct Target Ther*, **2023**, 24, 435.

Acknowledgments: This project has received funding from the European Union's Horizon Europe research and innovation program, grant agreement No 101058570 (RELIANCE).

**Optimization of Self-Healing and Anticorrosive Properties of Waterborne Polyurethane Coatings for the Protection of Metallic Artworks**

Elodia Spinelli<sup>1,2</sup>, Federico Oliviero<sup>3</sup>, Zhanhua Wang<sup>4</sup>, Hesheng Xia<sup>4</sup>, Gennaro Gentile<sup>3</sup>, Giovanna Buonocore<sup>1</sup>, Marino Lavorgna<sup>1</sup>, Silvia Licoccia<sup>2,3,5</sup>

<sup>1</sup> Institute of Polymers, Composite and Biomaterials, National Research Council of Italy, Portici (NA), Italy

<sup>2</sup> Department of Chemical Science and Technologies, University of Rome Tor Vergata, Rome, Italy

<sup>3</sup> Centre for Nanosciences, Nanotechnologies & Instrumentation (NAST), University of Rome Tor Vergata, Rome, Italy

<sup>4</sup> State Key Laboratory of Advanced Polymer Materials, Polymer Research Institute, Sichuan University, Chengdu, China

<sup>5</sup>Institute of Polymers, Composite and Biomaterials, National Research Council of Italy, Pozzuoli (NA), Italy

Email presenting author: [elodia.spinelli@students.uniroma2.eu](mailto:elodia.spinelli@students.uniroma2.eu)

Metallic works of art are particularly vulnerable to corrosion processes, which can compromise their structural integrity and historical value. A promising conservation strategy involves the design of multifunctional polymeric coatings that combine barrier and active corrosion inhibiting properties, while maintaining transparency, reversibility, and long-term stability against degradative agents. [1] Waterborne polyurethane matrices (WPU) are especially attractive thanks to their structural tunability and the possibility of introducing intrinsic self-healing properties, which allow coatings to restore after mechanical damage, providing long-term protection. [2] Additionally, the use of WPU as aqueous dispersions eliminate the need of toxic organic solvents, reducing the environmental impact associated with traditional solvent-based coatings. [3,4] In our work, WPU formulations, previously developed from Sichuan University, were optimized to enable self-healing at reduced temperatures while enhancing the protection of bronze surfaces. The addition of polyethylene glycol (PEG) increased polymer mobility, facilitating repair of surface scratches at low temperature, compatible with metallic artworks. Furthermore, benzotriazole was incorporated in the PEG modified WPU matrix as an active corrosion inhibitor. Accelerated corrosion tests demonstrated that PEG-modified coatings effectively preserved surface integrity, confirming their enhanced anticorrosion performance compared to the unmodified WPU coatings. These results highlight the potential of tailored WPU-based systems as environmentally friendly self-healing coatings for the long-term conservation of metallic artworks.

## References

- [1] F. Olivieri, F. Scherillo, R. Castaldo, M. Cocca, A. Squillace, G. Gentile, M. Lavorgna, ACS Applied Polymer Materials, 5, no.8 (2023): 5917-5925.
- [2] Ren S. , Zhou W., Song K., Gao X., Zhang X., Fang H., Li X., Ding Y., Progress in Organic Coatings 2023, 180.
- [3] C. Yu, M. Salzano de Luna, A. Russo, I. Adamiano, F. Scherillo, Z. Wang, X. Zhang, H. Xia, and M. Lavorgna, Adv. Mater. Interfaces 2021, 8, 2100117.
- [4] M. Salzano de Luna, Adv. Mater. Interfaces 2022, 9, 2101775.

# eXpanding CHEMistry: implementing excellence in research and teaching

X-CHEM III year Meeting, December 18<sup>th</sup> 2025

Department of Chemical Science and Technologies

*Evaluating Force-Field Refinements in RNA Molecular Dynamics: A Comparative Analysis of OL3 and CMAP Corrections in the HuR–Aptamer Complex*

Fabio Giovanni Tucci<sup>1</sup>, Alice Romeo<sup>1</sup>, Davide Pietrafesa<sup>1</sup>, Federico Iacovelli<sup>1</sup>, Mattia Falconi<sup>1</sup>

<sup>1</sup>Department of Biology, University of Rome “Tor Vergata”, Via della Ricerca Scientifica 1, 00133 Rome, Italy

Email presenting author: fabio.giovanni.tucci@uniroma2.it

This study employs computational chemistry approaches to investigate the impact of force-field refinements on RNA molecular dynamics (MD) simulations. We compare the widely used OL3 force field<sup>1</sup> with its CMAP-refined variant (OL3+CMAP)<sup>2</sup> using a biologically relevant model: the HuR protein bound to a 27-nucleotide single-stranded RNA (ssRNA)<sup>3</sup>. Due to its intrinsic flexibility, this system serves as a valuable benchmark for assessing the accuracy and reliability of RNA simulations.

Using extensive MD sampling (500 ns per replica), we assessed structural stability and conformational behavior through RMSD, RMSF, PCA, and eRMSD analyses. Our results reveal a clear trade-off: although OL3+CMAP enhances conformational diversity, it also introduces significant drawbacks, including poor convergence, excessive terminal fluctuations, and technical instabilities. In contrast, OL3 maintains stable trajectories and yields a reproducible conformational ensemble.

While local interactions (stacking and pairing) remain broadly comparable between force fields, the overall robustness of OL3 outweighs the increased heterogeneity introduced by the CMAP correction for this class of single-stranded RNA architectures. These findings provide practical guidance for modeling protein–RNA complexes, highlighting OL3 as the more reliable option pending further validation through advanced torsional analyses.

## References

- 1 M. Zgarbová, M. Otyepka, J. Šponer, A. Mládek, P. Banáš, T. E. Cheatham and P. Jurečka, *Journal of Chemical Theory and Computation*, 2011, **7**, 2886–2902.
- 2 J. Chen, H. Liu, X. Cui, Z. Li and H.-F. Chen, *Journal of Chemical Information and Modeling*, 2022, **62**, 372–385.
- 3 D. Pietrafesa, A. Romeo, F. G. Tucci, P. Fiorani, F. Iacovelli and M. Falconi, *J. Chem. Inf. Model.*, 2025, **65**, 11158–11172.