The 1st CIVIS3i-UAM Postdoctoral meeting

25th April 2024

Universidad Autónoma de Madrid
C/ Francisco Tomás y Valiente 7,
Facultad de Ciencias
Seminar room 310 – Modulo 0

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[THE BOOK OF ABSTRACTS]

FOREWORD

The 1st CIVIS3i-UAM Postdoctoral meeting has been hosted at the Facultad de Ciencias, Universidad Autónoma de Madrid, and organized in coordination with the CIVIS3i office in Aix-Marseille University. Our main aim has been to provide a forum for discussion, to facilitate integration, and to bring together researchers from the CIVIS3i postdoctoral programme. The meeting (in person) was held over a day, April 25 (Thursday) 2024 in Madrid, Spain. The meeting included a seminar session with five presentations given by the postdoctoral fellows of the 2nd CIVIS3i call hosted at the Universidad Autónoma de Madrid. Additionally, we must sincerely thank the participation of Dr. Rafaella Lenoir-Importa, Local Contact Point, and the presence of Clara Gomez Zapatero, member of the European Research Office at the UAM, who contributed to clarify questions related to the implementation of the postdoctoral programme, helping to the success of the meeting. We tried hard to ensure that the meeting would be well organized. We hope that it met the expectations. We are grateful to the speakers and the participants for their thought contributions.

Felipe Zapata Abellán, Ph. D.
On behalf of the Organizing Committee

Universidad Autónoma de Madrid
Departamento de Química

LIST OF PARTICIPANTS

Name	Department	Contribution
Luca Volpi	Departamento de Historia Antigua, Historia Medieval y Paleografía	Speaker
Eduardos Loukopoulos	Departamento de Química Inorgánica	Speaker
Elia Romera Figueroa	Departamento de Filología	Speaker
Ruth Helena Tichauer	Departamento de Física Teórica de la Materia Condensada	Speaker
Felipe Zapata Abellán	Departamento de Química	Organizer & Speaker
Anael Ben-Asher	Departamento de Física Teórica de la Materia Condensada	Participant
María Jesús Cabrera Afonso	Departamento de Química Orgánica	Participant
Rafaella Lenoir-Impronta	Local Contact Point, CIVIS3i Programme Universidad Autónoa de Madrid	Participant
Clara Gomez Zapatero	European Research Office, Universiad Autónoma de Madrid	Participant

ORAL PRESENTATION

EnEAp – Endangered Earthen Architecture project.
Ideas, Methodologies and Perspectives for the Conservation and Restoration of Archaeological Earthen Masonries in Western Asia.

Luca Volpi*

Departamento de Historia Antigua, Historia Medieval y Paleografía, Universidad Autónoma de Madrid

Conservation of archaeological earthen masonries is a challenging task. Earthen architectures deteriorate in a short period of time once exposed to weathering and other decay agents. Their conservation is a crucial point of every cultural heritage programme where earthen masonries are attested, and it also has ethical and philosophical issues. Selected area of the project is the Western Asia, a region where the use of earthen masonries was substantial due to the climatic and environmental conditions of the area and still is. The aim of the EnEAp project is to investigate the possibilities of enhancing the durability and strength of mudbricks against weathering and other decay agents using chemical stabilising materials that are sustainable, green, and ecologically friendly. However, to reach this point, preparatory studies are performed in order to deepen the knowledge of the climatic and environmental conditions of the area, and the natures of the raw materials used. Two approaches, together with their methodologies and limitations, are considered in this presentation: the first one is a comparative approach to the conservation and restoration analysis of archaeological earthen architecture in Western Asia using environmental and climatic data. The second one is the possibility to directly investigate the nature of the mudbricks through petrographic, chemical, mineralogical, mechanical and hydrographic tests.

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ORAL PRESENTATION

Development of smart porous materials as advanced sorbents of emerging water pollutants

Eduardos Loukopoulos*

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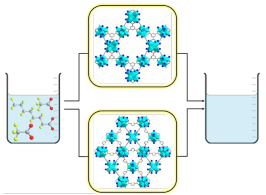
Water contamination is an issue of global concern and importance, aggravated by the emergence of man-made pollutants with high toxicity on human and aquatic organisms. Some of these contaminants have become a key priority of worldwide directives and regulations, as their chemical nature makes them extremely resistant to conventional wastewater treatment methods [B. Trang et al. *Science*, **2022**, 377, 839-845.]. Funded by the CIVIS3i fellowship programme, the AQUASORB project aims to overcome existing limitations by developing targeted, functionalized porous materials that can efficiently capture these pollutants through adsorption-based technologies. In this talk, the main principles behind the project will be presented, along with initial results on the enhanced capture of per- and polyfluoroalkyl substances (PFAS) (Figure 1).



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ORAL PRESENTATION

My Four Key Words: Performance, Music, Gender, Memory

Elia Romera Figueroa*

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Universidad Autónoma de Madrid

This presentation offers an overview of my research in countercultural uses of music and performance in 20th and 21st century Spain. I am currently at work on my forthcoming book, “Gendering Anti-Francoism: Cantautoras in Spain (1952–1986),” which explores how Iberian female singer-songwriters engaged with the anti-Franco struggle during the dictatorship and the transition to democracy. In this presentation, I will share a more contemporary example of my work, an essay I published in English in 2020 and am now in the process of translating to Spanish as a book chapter. The article in English was titled, "Voiced Postmemories: Rozalén’s “Justo” as a Case Study of Singing, Performing, and Embodying Mourning in Spain." I will use this case study to offer a glimpse of my present work.

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ORAL PRESENTATION

QOMQER - Quantum Optics Meet Quantum chEmistRy

Ruth Helena Tichauer*

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Universidad Autónoma de Madrid

In an ever growing society with ever increasing communication needs, low energy consumption devices that process information in a fast, robust and secure manner are highly desirable, with photonic circuits holding a great potential owing to their reduced losses and fast operation speed. Because of their outstanding properties and ease in production, organic photoactive molecules could be integrated in such circuits and function as the signalling processing elements. However, the photo physical properties of these type of molecules are dramatically affected by its material and electromagnetic environment. To asses the extent of these changes, my project aims at merging Quantum Optics and Quantum Chemistry approaches in a molecular dynamics framework to perform simulations of bright emitters, within their material environment, placed in nano-photonic structures. In this manner, it will be possible to study the photo-dynamics of emitters coupled to light with unprecedented accuracy in the description of both the complex material and electromagnetic fields emerging in the vicinity of nanostructures. The fundamental understanding on the excited state dynamics of the emitter in such conditions, has the potential to pave the way for the optimisation and design of devices based on molecule-nanophotonic components.

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ORAL PRESENTATION

RTDmol - Relativistic Time-Delays in molecules

Felipe Zapata Abellán*

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As suggested by recent experimental and theoretical works, core-level molecular photoionization time-delays may give us atom-resolved information about the potential and the geometry of the molecule [Rist *et al. Nat. Commun.* 12, 6657 (2021); Tamura *et al. J. Phys. B: At. Mol. Opt. Phys.* 55, 10LT01 (2022)]. From a theoretical perspective, in order to be able to reproduce core-level photoionization in molecules containing heavy atoms, a relativistic treatment is required. However, a practical resolution of the relativistic molecular problem is not trivial and sophisticated tools have to be implemented in order to avoid the apparition of the so-called "spurious states" in the spectrum of positive (electron) energies. Although very accurate methods have been proposed in the past, they are not able to handle molecular photoionization processes. On the contrary, the B-spline Galerkin method, previously implemented to study photoionization of heavy atoms [Zapata *et al. Phys. Rev. A* 105, 012802 (2022)], is an ideal method that can be extended to solve the 4-component two-center Dirac equation in many-electron molecules. In this sense, following previous implementations in the context of non-relativistic molecular calculations, a least squares B-spline approach can be used to determine the relativistic continuum solution. Here we present an overview of the derivation and the numerical performance of our relativistic methodology specially designed to explore molecular photoionization processes from inner shells [Zapata *et al.* (in progress)].

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GROUP PICTURE

CIVIS3i-UAM fellows, Facultad de Ciencias UAM 25th April 2024

[María Jesús Cabrera Afonso, Anael Ben-Asher, Elia Romera Figueroa and Eduardos Loukopoulos]
[Luca Volpi, Rafaella Lenoir-Impronta, Ruth Helena Tichauer and Felipe Zapata Abellán]