Interview of Dr. Emmanouel Klontzas, Associate Researcher, TPCI/NHRF

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Mr. Klontzas, you belong to the Sector of Theoretical and Computational Chemistry and Physics of the TPCI/NHRF as Associate Researcher. We would like to talk to us about this area of research. What are its main activities?

The Theoretical and Computational Chemistry and Physics section of the TPCI/NHRF is one of the most dynamic areas of the Institute and is active in the field of study with theoretical and computational techniques of the physical and chemical properties of atoms, molecules and materials. This is achieved through the extensive use of computers and high-quality software that combines knowledge of different subjects such as physics, theoretical chemistry, computing and mathematics. The progress of the sector is directly related to the evolution of computers and the corresponding software. Now, it is possible to study systems consisting of a few tens to millions of people, depending on the computational methods to be used. Depending on the problem we have to deal with each time, we should also choose the appropriate computing method, which will give us accurate results in a reasonable amount of time. The choice also depends on the size of the system and the time evolution of the phenomenon we want to study. It often takes more than one method to get the best picture of the chemical system we are studying. These methods include calculations of the electronic structure of matter, molecular mechanics/dynamics techniques and lastly the use of machine learning techniques.

Tell us a bit about the areas of application or services that emerge from the growing know-how in this field.

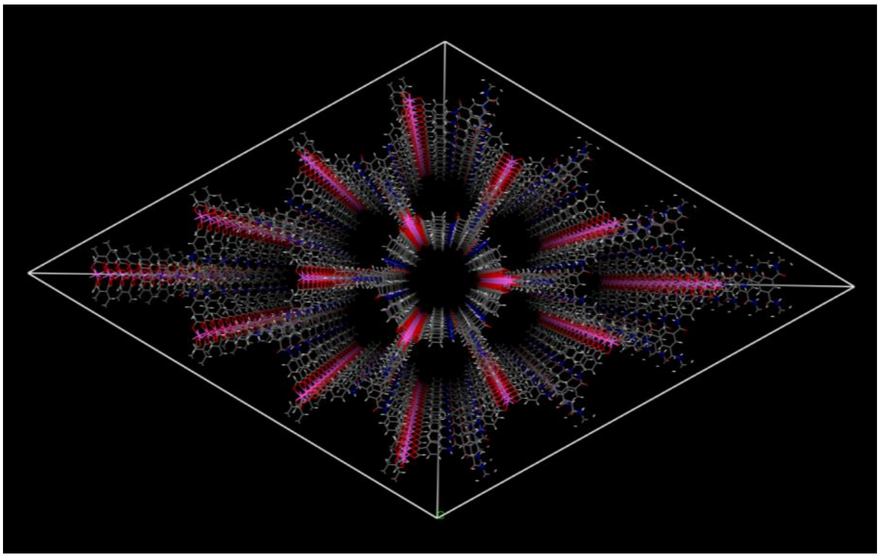
Research carried out in this field serves a deeper understanding of the mechanisms of phenomena observed in a system under study and provides the capability to predict a wide range of properties of molecules and materials with great accuracy. Computational methods often help to interpret the results of an experimental process. Sometimes they predict properties that would be difficult to be measured experimentally. Important work is being carried out towards investigation of the enhanced conditions of molecules and materials. Also important work is done in the spectroscopic characterization of both organic and inorganic chemical systems. Other areas of application are the study of chemical reaction mechanisms and the adsorption of chemicals on surfaces and porous materials.

What do you consider as challenges/difficulties for a researcher today?

The challenges facing a researcher today are many, at different levels, and it takes a lot of effort to be able to be met. The most important challenge is that we are called upon to serve the needs of society and to solve the problems it faces. Beyond that, the research we produce has to be competitive at international level and highly impactful in the sector. Especially in the cutting-edge fields, the researcher in Greece is called upon to "team up" with corresponding teams around the world, without having the same tools to generate innovative ideas and to implement them very quickly. The researcher should then be able to attract the appropriate funding to carry out his research and be able to set up his own research team and be provided of the logistical infrastructure and supplies they need. The lack of planning in the announcement of funding for research projects contributes negatively in this area but gradually the situation appears to be changing. Another challenge is to disseminate the knowledge and results of the research work carried out to society. Although there are specific channels of communication through which the results of the research project become known to the scientific community, e.g. through publications in international journals and scientific conferences, there are no corresponding channels for citizens and students. Despite the adversity that exists, Greek researchers are doing well by presenting important published work, attracting significant funding from competitive programs and contributing significantly to their respective research fields.

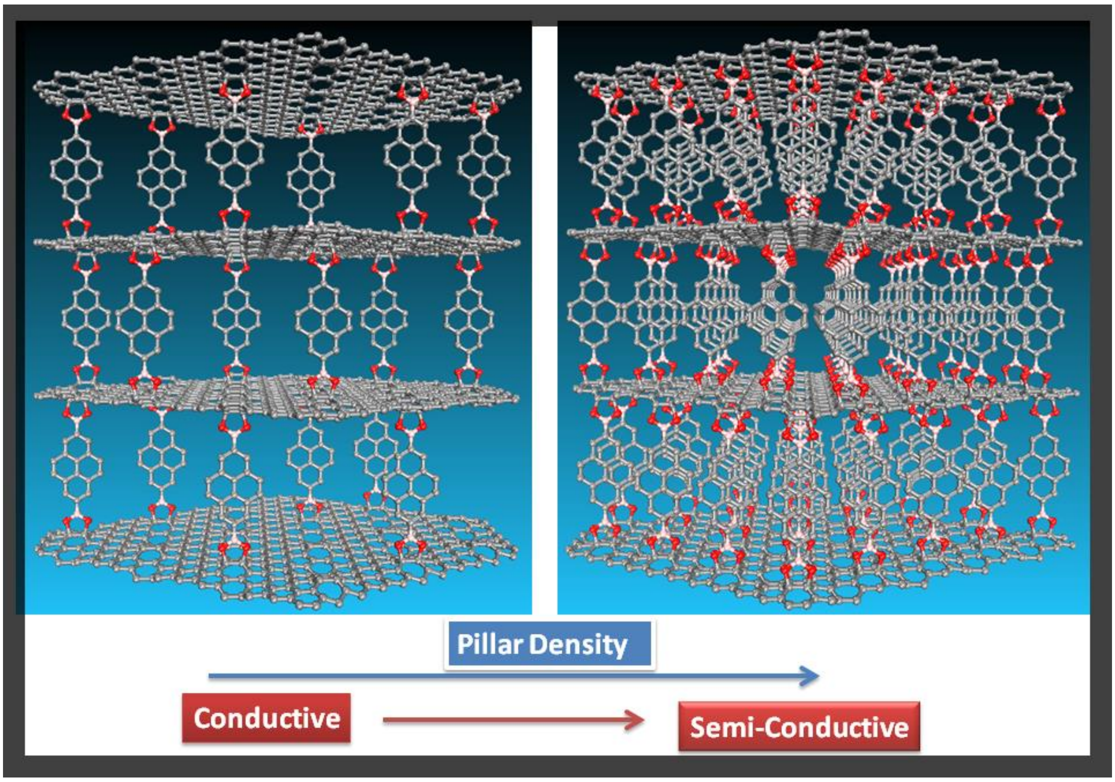
Is there a cutting edge field you are currently focusing on? What are your future goals regarding this?

My research interests currently focus primarily on the design of porous materials for applications related to the environment and energy using computational chemistry. Porous are solid materials which have an extensive network of pores, such as a sponge, with one of the most well-known examples being zeolites and activated carbons. In our studies, we use both traditional porous materials and materials that belong to new categories and have greater potential, such as the metal-organic skeletal materials of the MOF (Metal-Organic Frameworks) and ZIF (Zeolite Imidazolate Frameworks) families. For each of the applications we are designing porous materials for, specific requirements must be fulfilled which we should take into account. Part of our research is concerned with the effects of climate change and environmental pollution on human activities, which are little known. We try to help mitigate its effects and reverse the whole situation by designing materials that can selectively capture gases that contribute to the greenhouse effect so that they are not released into the environment, such as carbon dioxide or sulphur hexafluoride. The new porous materials we design make the whole process of capturing and storing such gases more efficient and energy efficient.



Graphic image of a MOF structure with one-dimensional porous channels.

At the same time, with the above research activity, we are also participating in a research project funded by the Hellenic Foundation for Research and Innovation, which deals with the design of new stamped graphene structures with controlled electronic and mechanical properties. In this program, we are studying through computational techniques how the alteration of the chemical composition and some structural characteristics of graphene can cause changes in the electrical behavior of these materials by converting them, for example, into conductors in semiconductors. In addition, we are interested in learning how their electrical properties change when they are deformed in different types and directions.



Alteration of the electrical properties of graphene-based stamped materials by varying the density of pylons.

We have also recently begun to work on issues related to moisture capture by the atmosphere and selective capture of organic pollutants by aqueous solutions. In the first case, we aim to design porous materials that are capable of capturing a significant amount of moisture from the atmosphere in areas without water and then able to return it to the wet phase. The ability of these materials to bind water is directly related to both the properties of these materials and the conditions under which they will be required to cope, such as relative humidity and temperature over a 24-hour period and their performance should be optimized under the prevailing conditions. In the latter case, we are studying how certain materials in the MOF family can be used to capture organic pollutants that do not easily degrade in nature and remain for a long time in aquatic systems. Such organic pollutants, for example, are phenols, various antibiotics, and even substances used in sunscreens. Our goal is to bind them into porous materials and then break them down into smaller, less harmful, chemical compounds. The research is to be funded by the State Scholarship Foundation (IKY) through the action of postdoctoral researchers.