# XXXV Panhellenic Conference on Solid State Physics and Materials Science

**September 26-29, 2021**
**Virtual Conference**
http://xxxv-ssm.inn.demokritos.gr/

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School on

# Theoretical/Computational Condensed Matter Physics and Materials Science

Sunday 26th September 2021

12:00 **Opening**
**Prof. Leonidas Tsetseris**
National Technical University of Athens

12:00 -13:45 **Machine learning potentials for complex aqueous systems made simple**
**Dr. Christoph Schran**
Yusuf Hamied Department of Chemistry, University of Cambridge (UK)

13:45-15:00 Lunch Break

15:00-16:45 **Quantum information processing with solid-state qubits**
**Prof. Sophia Economou**
Department of Physics, Virginia Tech (USA)

16:45-17:00 Coffee Break

17:00-18:45 **Role of electron interactions and topological superconductivity in Weyl-type materials**
**Prof. Efstratios Manousakis**
Department of Physics, Florida State University (USA) and Department of Physics, National and Kapodistrian University of Athens (GREECE)

18:45 **Closing**
**Prof. Leonidas Tsetseris**
National Technical University of Athens

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## SPEAKERS

**Prof. Sophia Economou**
Department of Physics,
Virginia Tech (USA)

Prof. Economou obtained her PhD in 2006 from the University of California San Diego. After that, she spent nine years at the US Naval Research Lab, first as a National Research Council Postdoctoral Fellow, and then as Research Staff. She joined Virginia Tech in 2015 where she is currently a Professor of Physics and the Hassinger Senior Fellow of Physics at Virginia Tech. She focuses on theoretical research in quantum information science, including quantum computing, quantum communications, and quantum simulation algorithms.

**Prof. Efstratios Manousakis**
Department of Physics,
Florida State University (USA) and
Department of Physics,
National and Kapodistrian University of Athens (GREECE)

Dr. Manousakis received his Ph. D. in Theoretical Physics, in July 1985, from the University of Illinois at Urbana-Champaign (First Ross J. Martin Award for his thesis). After a Post-Doctoral Research position at the Center for Theoretical Physics at the Massachusetts Institute of Technology (1985-1987) and at the Supercomputer Computational Research Institute (1987-88), he joined the Physics Department of the Florida State University (FSU) (1988). He received the PAI Award for Excellence in Teaching and Research (1998) and the Developing Scholar Award (1990) from FSU. Presently, he is Professor of Physics at the University of Athens and he is the Donald Robson Professor of Physics and holds the title of Distinguished Research Professor at FSU. He was named Fellow of The American Physical Society in 2002, Fellow of the Institute of Physics in 2008, and Fellow of American Association for Advancement of Science in 2018. Dr Manousakis' group develops and applies computational and theoretical methods to study novel collective behavior in certain quantum many-body systems which arises because of strong correlations among the fundamental microscopic degrees of freedom. Examples of such systems are: (a) Superconductors and Strongly Correlated Electrons, (b) Superfluids, (c) Electrons in Solids and The Two-Dimensional Electron Gas, (d) Quantum Phase Transitions in Atomically Thin Films and (e) Phase Transitions in Restricted Geometries and Finite Size Scaling (f) Role of correlations in topological materials

**Dr. Christoph Schran**
Yusuf Hamied Department of Chemistry,
University of Cambridge (UK)

Christoph Schran received his PhD in chemistry from the Ruhr-Universität Bochum, Germany in 2019 where he worked with Dominik Marx on hydrogen bonded systems solvated by superfluid helium. During this time he visited the École normale supérieure, Paris and was a visiting graduate student in the Markland group at Stanford University. For his postdoctoral work, he moved to the University of Cambridge working with Angelos Michaelides as a fellow of the 'Alexander von Humboldt' foundation. His research interests include the understanding of hydrogen bonded systems and their modelling by machine learning techniques.

# Syllabus

## Machine learning potentials for complex aqueous systems made simple

Simulation techniques based on accurate and efficient representations of potential energy surfaces are urgently needed for the understanding of complex materials such as solid-liquid interfaces. In this lecture, the principles of modern machine learning potentials will be outlined, explaining how the structure-energy relation required for molecular simulations can be represented by different approaches both based on neural networks or kernel based methods. Further emphasis will be on the efficient development and validation of such models. Finally, example applications of machine learning potentials for the understanding of complex materials will be presented to ultimately guide material design. Such machine learning models provide a straightforward and uncomplicated but accurate extension of simulation time and length scales for complex systems.

## Quantum information processing with solid-state qubits

I will give a broad introduction to quantum information processing and focus on implementations with solid-state systems. Specifically, I will discuss spin-based quantum computing with quantum dots and optically active solid-state spin systems for quantum networks. I will present the physical mechanisms and control techniques for the implementation of quantum operations as well as the challenges that limit quantum information applications. I will also highlight interesting recent experiments from some of the leading groups in the field.

## Role of electron interactions and topological superconductivity in Weyl-type materials

During the last two or three decades topology is becoming a powerful tool to characterize the electronic properties of materials. Most of the effort has been invested looking from a single-particle point of view, namely, without including the role of electron correlations. Here, we will first review the concepts of the topological insulator and of Dirac and Weyl materials of various types. Next, we will give theoretical examples of Weyl semimetals and of Weyl nodal-ring semimetals. The nature of the surface states will be discussed. We will then discuss examples of electron interactions which lead to non-topological and topological superconductivity in such Weyl systems, including the formation of Majorana and Bogoliubov-Weyl surface states. Finally, we will also give examples where the effect of strong Coulomb correlations is to destroy the Weyl behavior.