# SYES 1: Electronic Structure Theory for Quantum Technology

Time: Friday 9:30–12:15 Location: H1

**Invited Talk** SYES 1.1 Fri 9:30 H1

**Ab-initio Design of superconductors** — •Lilia Boeri — Physics Department, Sapienza University, Rome, Italy

Over the last ten years, ab-initio methods for superconductivity and crystal structure prediction have seen a substantial advancement, opening the concrete possibility of designing new conventional superconductors completely in silico. The most spectacular demonstration of the power of this approach is the prediction of high-temperature conventional superconductivity in compressed sulfur hydride, which started the so-called hydride rush towards room-temperature superconductivity.[1] However spectacular these discoveries might be, bridging the gap with applications requires devising new strategies to realize high-Tc at more accessible pressures [2], and understanding the origin of superconductivity in seemingly simple materials, like Hg and NbTi. Finally, I will addressed the challenges that the community needs to address after recent reputation breaches due to false claims of room-temperature superconductivity [3]. [1] J. A. Flores-Livas, L. Boeri, A. Sanna, G. Profeta, R. Arita, M. Eremets, Physics Reports 856, 1-78 (2020). [2] R. Lucrezi, S. di Cataldo, W. von der Linden, L. Boeri and Christoph Heil, NPJ Computational Materials, 8, 119 (2022). [3] P. Ferreira , L. J. Conway, A. Cucciari, S. Di Cataldo, F. Giannessi, E. Kogler, L. T. F. Eleno, C. J. Pickard, C. Heil and L. Boeri, Nature Comm. 14, 5367 (2023)

**Invited Talk** SYES 1.2 Fri 10:00 H1

**Topological superconductivity from first principles** — Bendegúz Nyári[1,2], András Lászlóffy[3], Levente Rózsa[3,2], Gábor Csire[4], Balázs Újfalussy[3], and •László Szunyogh[2,1] — [1]HUN-REN BME Condensed Matter Research Group, Budapest, Hungary — [2]Budapest University of Technology and Economics, Budapest, Hungary — [3]HUN-REN Wigner Research Centre for Physics, Budapest, Hungary — [4]Materials Center Leoben Forschung GmbH, Leoben, Austria

Magnetic chains manufactured on superconductors are possible candidates for fault tolerant quantum computing architectures. Due to the interplay of magnetism and superconductivity these systems are suitable to host topological zero-energy end states, the so-called Majorana Zero Modes (MZM). In this talk we present a first-principles approach suitable to study atomic chains by employing an embedding technique within the Multiple Scattering Theory, combined with the solution of the Bogoliubov–de Gennes equations. In case of Fe chains on an Au monolayer on Nb(110) we show that the formation of MZMs is supported in a broad range of spin-spiral states. Through computer experiments we also demonstrate the emergence of topological fragmentation and simulate the shifting of MZMs within the nanowire. Our computational method allows for calculating the one-dimensional band structure of infinite chains which provides a clear picture to analyze the topological properties of Shiba bands. The band structure is calculated and compared with the quasiparticle interference spectrum for Mn chains on Nb(110) and Ta(110).

**Invited Talk** SYES 1.3 Fri 10:30 H1

**First-principles study and mesoscopic modeling of two-dimensional spin and orbital fluctuations in FeSe** — •Myrta Grüning[1,2], Abyay Ghosh[1], and Piotr Chudzinski[1,3] — [1]Centre for Quantum Materials and Technologies, Queen's University Belfast, Belfast, Northern Ireland (UK) — [2]European Theoretical Spectroscopy Facility — [3]Institute of Fundamental Technological Research, Polish Academy of Sciences, Warsaw, Poland

FeSe is the simplest quasi-two-dimensional iron chalcogenide superconductor, yet its phase diagram exhibits exotic phases like superconductivity, spin density wave, and nematicity, which are intensely studied in condensed matter physics. Understanding the interaction of orbital and spin degrees of freedom is key to explaining FeSe's diverse phases. Using density-functional theory within the generalized gradient approximation, we calculated the structural, electronic, and magnetic properties of FeSe in its tetragonal phase. First, we explored how the d-band bandwidths at the Fermi energy evolve with corrections and long-range magnetic orders. Introducing striped or staggered dimer antiferromagnetic order significantly reduced the bandwidth overestimation seen at the generalized gradient approximation level, aligning more closely with experimental data. Next, we examined the magnetic formation energy for ferromagnetic and antiferromagnetic orders, under pressures up to 6 GPa and derived bilinear and biquadratic spin-exchange energies. We uncovered non-trivial spin-exchange behavior dependent on magnetization and proposed a field-theory model linking this to strong two-dimensional spin-orbital fluctuations.

**15 min. break**

**Invited Talk** SYES 1.4 Fri 11:15 H1

**Non-collinear magnetism in 2D materials from first principles: Multiferroic order and magnetoelectric effects.** — •Thomas Olsen — Department of Physics, Technical University of Denmark

We present a systematic classification of the magnetic ground states in hundreds of two-dimensional (2D) materials. Non-collinear order is shown to be abundant and may typically be represented by planar spin spiral ground states. We discuss a range of physical effects associated with non-collinear order and take specific materials as examples. The $Ni(Cl,Br,I)_2$ compounds exhibit type II multiferroic order where the spontaneous polarization is induced by spiral order and we discuss the subtleties associated with the calculation of the polarization from first principles. The breathing Kagomé compounds $Nb_3(Cl,Br,I)_8$ are pyroelectric and have spiral ground states with ordering vectors that couple strongly to out-of-plane external electric fields. Finally we discuss a set of 2D altermagnets and analyse the important role of spin-orbit coupling with respect to the band structure, magnons and non-collinearity.

**Invited Talk** SYES 1.5 Fri 11:45 H1

**Spin-phonon and magnon-phonon interactions from first principles** — •Marco Bernardi — Caltech

Electron-phonon interactions have become a major research focus in first-principles electronic structure calculations. This talk discusses our recent efforts to include the spin degree of freedom in this framework.

First, I will present precise predictions of spin-phonon interactions and electron spin relaxation using a new approach that unifies the description of spin-flip and precession mechanisms. Second, I will describe an approach to compute magnon-phonon interactions and the associated magnon relaxation times and mean-free paths, focusing on results for 2D ferromagnetic materials. Our calculations shed light on which phonon modes couple more strongly with free spins and magnons and limit their transport, providing valuable microscopic insight for applications in spintronics and spin-based quantum technologies.

To conclude, I will highlight new frontiers of this research, including data-driven compression of electron-phonon and spin-phonon interactions and extending these methods to the strong spin-phonon coupling regime. Advances in the Perturbo code enabling these calculations will also be discussed.