TT 91: Superconductivity: Theory II

Time: Thursday 17:30–18:30 Location: HSZ/0101

TT 91.1 Thu 17:30 HSZ/0101

Superconducting length scales and currents from first principles — Mitsuaki Kawamura[1], Takuya Nomoto[2], •Niklas Witt[3], and Ryotaro Arita[4,5] — [1]Yokohama National University, Japan — [2]Tokyo Metropolitan University, Japan — [3]JMU Würzburg, Germany — [4]University of Tokyo, Japan — [5]RIKEN CEMS, Japan

Superconducting length scales, namely the coherence length and the penetration depth, as well as critical currents, are central to the performance of superconductors but remain challenging to obtain from first principle calculations. While density functional theory for superconductors (SCDFT) has been widely used to predict transition temperatures, magnetic and current related superconducting properties are far less explored.

We present a fully ab initio implementation of a recently introduced method [1] within SCDFT, which gives access to superconducting length scales and depairing currents by introducing a finite-momentum pairing constraint. The approach has been integrated into the open-source superconducting-toolkit (SCTK) [2] and applied to representative elemental, alloy, and high-pressure hydride superconductors. The results demonstrate a viable route to predicting magnetic superconducting properties directly from electronic structure calculations.

[1] N. Witt et al., npj Quantum Mater. 9, 100 (2024)
[2] M. Kawamura et al., Phys. Rev. B 101, 134511 (2020)

TT 91.2 Thu 17:45 HSZ/0101

Cavity-control of the Ginzburg-Landau stiffness in superconductors — •Vadim Plastovets and Francesco Piazza — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Confining light around solids via cavities enhances the coupling between the electromagnetic fluctuations and the matter. We predict that in superconductors this cavity-enhanced coupling enables the control of the order-parameter stiffness, which governs key length scales such as the coherence length of Cooper pairs and the magnetic penetration depth. We explain this as a renormalization of the Cooper-pair kinetic mass caused by photon-mediated repulsive interactions between the electrons building the pair. This effect is generic for Bardeen-Cooper-Schriffer superconductors and is most pronounced in low-Tc materials. The strength of this effect can be tuned via the length of the cavity and we estimate it to be sizable for cavities in the infrared range.

TT 91.3 Thu 18:00 HSZ/0101

Influence of Cavity-Induced Polariton Formation on Superconductivity — •Paul Bodewei[1], Paul Fadler[1], and Michael A. Sentef[1,2] — [1]Institute for Theoretical Physics, University of Bremen/ Bremen Center for Computational Material Science — [2]Max Planck Institute for the Structure and Dynamics of Matter, CFEL, Hamburg

Cavities have emerged as a powerful tool for manipulating quantum materials, leveraging vacuum fluctuations to alter fundamental material properties. Recent experiments on the organic high-T_c κ-salts report a dramatic suppression of the superfluid density when those are coupled to a cavity [1]. The prevailing hypothesis for this suppression arises from a resonant coupling between the cavity modes and infrared-active molecular phonon modes in the κ-salt. However, the microscopic mechanism by which such cavity-induced phonon/polariton coupling alters superconductivity remains unknown. To gain further understanding on this, we focus on charge-transfer κ-salts with strong electronic correlations, which are well captured by a Hubbard model [2,3]. Building on that, our goal is to understand how the emergence of cavity-mediated phonon polaritons modifies the effective interactions (e.g. spin fluctuations [4] or mediated electron pairing), and thereby to examine how and why the superconducting state is suppressed.

[1] I. Keren, T.A. Webb, S. Zhang et al., arXiv:2505.17378 (2025)
[2] M. Buzzi et al., *Phys. Rev. X*, **10**, 031028 (2020)
[3] H. Menke et al., *Phys.l Rev. Lett.* **133** 136501 (2024)
[4] J. Schmalian, *Phys. Rev. Lett.*, **81**, 4232 (1998)

TT 91.4 Thu 18:15 HSZ/0101

Unraveling Quantum Effects of Flexible Molecules in Superfluid Solvents — •Katharina Leitmann[1], Harald Forbert[1,2], and Dominik Marx[1] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, GER — [2]Center for Solvation Science ZEMOS, Ruhr-Universität Bochum, 44780 Bochum, GER

Protonated methane (CH_5^+) is a fluxional molecule whose sensitivity to its environment makes it an excellent probe for low-temperature molecular interactions. We investigate CH_5^+ microsolvation in *para*-hydrogen clusters $(p\mathrm{H}_2)_n$ at low temperatures using two distinct simulation approaches: Ring Polymer Molecular Dynamics at 15 K to compute IR spectra and a hybrid simulation approach that combines Path Integral Molecular Dynamics for CH_5^+ and bosonic Path Integral Monte Carlo to establish Bose-Einstein statistics of the $(p\mathrm{H}_2)_n$ quantum solvation environment, subject to bosonic exchange at 1 K.

All simulations are based on highly accurate High-dimensional Neural Network Potentials and the IR spectra are computed using a Neural Network Dipole Moment Surface, both parameterized using CCSD(T) theory. Our simulations demonstrate stable solvation of CH_5^+ at least up to $n = 12$ $p\mathrm{H}_2$ molecules, which build the first solvation shell. We revealed that the structure of CH_5^+ is not significantly perturbed by the solvation with $p\mathrm{H}_2$. However, we found significant fluctuations in the large amplitude motion of CH_5^+ associated with partial hydrogen scrambling as a function of cluster size n. These dynamic influences are consistently observed in the IR spectra, underscoring the robustness of our findings across different methodologies and temperatures.