

**Theoretical and Physical Chemistry Institute
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ONLINE LECTURE

**“Understanding the supercritical state through
experiments and calculations”**

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Understanding the supercritical state through experiments and calculations

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In the first part of the talk, I will examine some of the distinctive properties of the supercritical state. Physics of supercritical state is understood to a much lesser degree compared to subcritical liquids. Carbon dioxide in particular has been intensely studied, yet little is known about the supercritical part of its phase diagram. I will show how by combining neutron scattering experiments and molecular dynamics simulations we can demonstrate the structural crossover between liquid-like and gas-like supercritical states at the Frenkel line [1]. The crossover was seen at pressure extending to 14 times the critical pressure and was evidenced by changes of the main features of the structure factor, pair distribution functions and coordination numbers. I will also discuss some studies on the supercritical mixtures of Xe-N₂ [2] and Ar-N₂ [3]. In the case of Xe-N₂, we studied PVT-data, diffusion and dynamics using classical MD calculations and depolarized Rayleigh scattering spectroscopy. In the case of Ar-N₂, PVT-data, diffusion and microscopic structure using classical molecular dynamics (MD) calculations and neutron scattering experiments were studied. Finally, we will discuss some current and future work on studies of supercritical systems of radicals [4].

References:

- [1] C. J. Cockrell, O. Dicks, L. Wang, K. Trachenko, A. K. Soper, V. V. Brazhkin, S. Marinakis, "Experimental and modeling evidence for structural crossover in supercritical CO₂", *Phys. Rev. E.*, **101**, 052109 (2020).
- [2] A. K. Soper, I. Skarmoutsos, J. Kłos, J. Samios, S. Marinakis, "A study of Ar-N₂ supercritical mixtures using neutron scattering, molecular dynamics simulations and quantum mechanical scattering calculations", *J. Mol. Liq.*, **290**, 111168 (2019).
- [3] D. Dellis, J. Samios, B. Collet, H. Versmold, J. Kłos, S. Marinakis, "An investigation of thermodynamic, microscopic structure, depolarized Rayleigh scattering, and collision dynamics in Xe-N₂ supercritical mixtures", *J. Mol. Liq.*, **245**, 42-51 (2017).
- [4] S. Marinakis et al., work in progress.