**Two-component dynamics and the liquid-like to gas-like crossover in water and other fluids at supercritical conditions**

**Prof. Giulio Monaco**

*Physics and Astronomy Department, University of Padova, Italy*

13 ottobre 2021 ore 15:00 – Piattaforma TEAMS

(codice: kopvp5w; per utenti esterni: <https://bit.ly/3D4Sz1q>)

info: [antonio.benedetto@uniroma3.it](mailto:antonio.benedetto@uniroma3.it); [luca.persichetti@uniroma3.it](mailto:luca.persichetti@uniroma3.it); [armida.sodo@uniroma3.it](mailto:armida.sodo@uniroma3.it);

Despite the technological importance of supercritical fluids, controversy remains about the details of their microscopic dynamics. Here, I will report on the molecular-scale dynamics in sub- to super-critical water studied with inelastic Xray scattering and molecular dynamics simulations. The obtained longitudinal current correlation spectra can be decomposed into two main components: a low-frequency (LF), gas-like component and a high-frequency (HF) component reminiscent of the longitudinal acoustic mode in ambient water. With increasing temperature, the hydrogen-bond network diminishes and the spectral weight shifts from HF to LF, leading to a transition from liquid- to gas-like dynamics with rapid changes around the Widom line. The molecular dynamics simulation studies are further extended to three more supercritical fluid systems - Si, Te, and Lennard-Jones fluid. The twocomponent behavior reported for water is observed in the intermolecular dynamics of all these systems, thus suggesting that it is likely universal. We find evidence to connect the liquidlike component dominating at lower temperatures with intermolecular bonding, and the component prominent at higher temperatures with free-particle, gas-like dynamics. The ratio between the components can be used to describe important properties of the fluid, such as its self-diffusion coefficient, in the transition region. Our results provide insight into the fundamental mechanism controlling the dynamics of supercritical fluids, and highlight the role of spatio-temporally inhomogeneous dynamics even in thermodynamic states where no large-scale fluctuations exist in the fluid.

**References**

**[1] P. Sun, J.B. Hastings, D. Ishikawa, A.Q.R. Baron, G. Monaco. Twocomponent dynamics and the liquidlike to gaslike crossover in supercritical water. Phys. Rev. Lett. 125, 256001 (2020).**

**[2] P. Sun, J.B. Hastings, D. Ishikawa, A.Q.R. Baron, G. Monaco. Universal twocomponent dynamics in supercritical fluids. arXiv preprint arXiv:2104.07732**