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Structural characterization of water networks

Liquid water, besides being fundamental for life on Earth, has long fascinated scientists due to several anomalies. Different hypotheses have been put forward to explain these peculiarities. The most accredited one foresees the presence in the supercooled region of two phases at different densities: the low-density liquid phase (LDL) and the high-density liquid phase (HDL). In a previous study [1], we proposed a new order parameter based on graph-theory, the total communicability [2], to identify these two forms in water networks at temperatures that cross the liquid-liquid coexistence line at 1950 bar. In [3], we analyzed the structure of the LDL and HDL phases at 1950 bar using consolidated global metrics from network theory. The results showed that these networks are only moderately complex, and that the lattice-like regular structure of the low-density phase is perturbed in the high-density form. More recently, we demonstrated that the total communicability can identify the two liquid phases also along the 1 bar isobar, along which there is no phase transition between LDL and HDL, but rather a continuous change in the amount of the two components with the temperature. Furthermore, we extended the analysis conducted in [3] to these 1 bar networks, confirming the moderate complexity of these water networks. Despite the moderate complexity, the total communicability is not only able to catch the changes in the networks that characterize the two phases, but is also computationally efficient compared to other centrality measures.

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Primary authors: Prof. BENZI, Michele (Scuola Normale Superiore); Prof. DAIDONE, Isabella (Department of Physical and Chemical Sciences, University of L'Aquila); FACCIO, Chiara (Scuola Normale Superiore); Dr ZANETTI-POLZI, Laura (Center S3, CNR-Institute of Nanoscience, Modena)

Presenter: FACCIO, Chiara (Scuola Normale Superiore)