Density forms of liquid water revealed by the Total Communicability of the corresponding graph

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In various parts of chemistry, graph theory has long been applied to create simple mathematical models of molecules and their links. Typically, the atoms (or the molecules) correspond to the graph nodes, and their chemical bonds correspond to the edges. In this talk, based on [2], we propose a new order parameter based on the Total Communicability to identify the low-density liquid (LDL) and high-density liquid (HDL) phases of liquid water. Although network-based approaches have been applied to the investigation of other water-related processes, the problem of determining the LDL and HDL phases using centrality measures has not been considered before. The Total Communicability [1] of a node v_i is defined as: $TC(v_i) = [e^{\beta A}\mathbf{1}]_\mathbf{i}$, where $\mathbf{1}$ is the vector of ones, A is the adjacency matrix of the network, and $\beta > 0$ is a parameter. This quantity has an interpretation in terms of walks on the graph, it takes into account the global properties of the network, and it can be computed efficiently using algorithms for computing the action of a matrix function on a vector, that is, for computing the vector $f(A)v$ for a matrix A (usually large and sparse), a vector v, and function f.

Joint work with M. Benzi, I. Daidone*, and* L. Zanetti-Polzi

References

[1] M. Benzi and C. Klymko, *Total communicability as a centrality measure*, Journal of Complex Networks, Volume 1, Issue 2, (2013), pp. 124–149.

[2] C. Faccio, M. Benzi, L. Zanetti-Polzi and I. Daidone, *Low, high and very-high density forms of liquid water revealed by a medium-range order descriptor*, arXiv preprint arXiv:2110.13747 (2021).