Topological Modeling of Proton Hopping on Hydrogen Bond Network in Liquid Water

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Abstract:
The proton conductivity in water largely depends on the topology of hydrogen bond network. Straightforward quantum mechanical calculation takes much computational cost to calculate the proton conductivity and the dynamics of the network in aqueous solution. To reduce the computational cost, we characterize the hydrogen bond network in liquid water as a dynamic directed graph from the calculation results of classical molecular dynamics, and analyze the dynamic and static properties of the network using the graph theory. Although the static structure of the hydrogen bond network is not free-scale, the dynamics has a free-scale property in time. We calculate the mean rate of Hamming displacement (MHD) in order to show the free-scale dynamics of the hydrogen bond network. The MHD is calculated as an ensemble average of Hamming distances between two network structures at different time steps. The MHD of the hydrogen bond network in liquid water to time becomes proportional to time with the exponent, 0.48. Furthermore, we construct a model of the proton hopping in liquid water as a random walk on the dynamic directed graph. We estimate the diffusion coefficient of proton and compare it with the experimental result.