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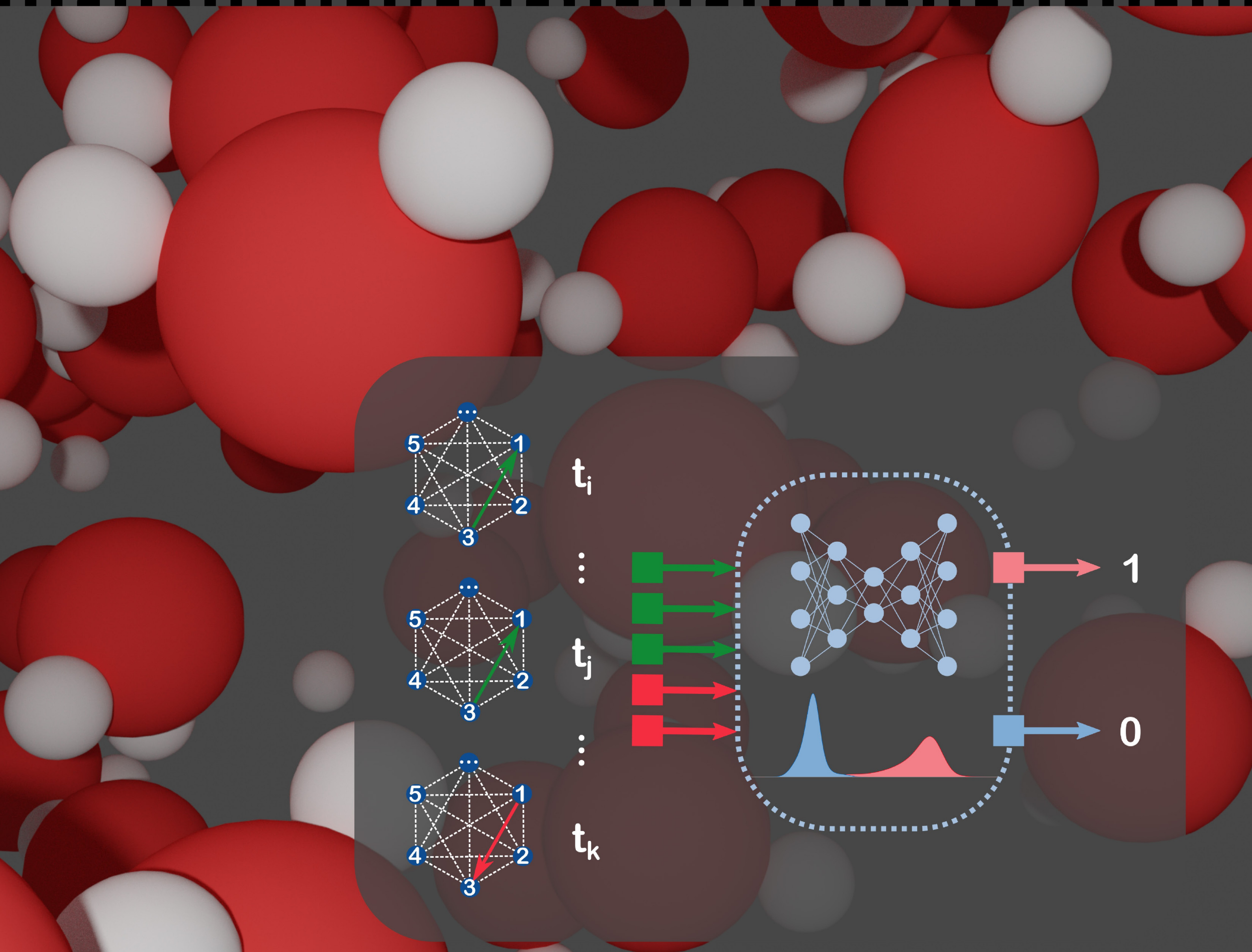
Front Cover:
Jie Huang, Gang Huang and Shiben Li
A Machine Learning Model to Classify Dynamic Processes in Liquid Water



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The front cover artwork is provided by the groups of Prof. Shiben Li (Wenzhou University, P.R. China) as well as Dr. Gang Huang (Institute of Theoretical Physics, Chinese Academy of Sciences, P.R. China). The image shows that characteristics of dynamic processes of water molecules in liquid water can be recognized and classified by a machine learning-based model if a graph representation is used to describe the hydrogen bond network. Read the full text of the Article at 10.1002/cphc.202100599.

What is the most significant result of this study?

Based on *ab initio* molecular dynamics (AIMD) simulations and a newly defined directed Hydrogen (H-) bond population operator, we designed a machine learning-based model to recognize different types of processes related to H-bonds in liquid water. This model may be used for other molecules and processes to recognize the characteristics of their dynamics.

Is your current research mainly curiosity driven or rather applied?

At first, we noticed that it's feasible to observe the different processes in the trajectory of simulated liquid water. As this type of process has received attention in theory, simulations, and experiments, then a natural question came to us: Is there a large number of interchange processes in liquid water? To answer this question, we developed a model to classify different types of dynamic processes in liquid water.

What was the biggest challenge on the way to the results presented in this paper?

Finding a suitable variable to monitor the dynamic processes in liquid water was one of the challenges we met. It should be sufficient to characterize the dynamic processes related to H-bonds, yet simple enough for us to handle the data. Fortunately, the directed H-bond population operator met our expectations. We could recognize different processes like interchange processes and diffusion processes easily just by analysing the time sequence of the directed H-bond population operator. Therefore, this variable played a key role in this work.

What future opportunities do you see in the light of the results presented in this paper?

The inspiration of viewing water as a network composed of many directed H-bonded rings makes it possible to study the complex H-bonded superstructures characteristic of liquid water. Therefore, extending our framework is promising, if reasonable variables to represent the properties of H-bonded rings are used. Besides, machine learning may be used to analyse extremely rapid processes. For example, the detection of high-density liquid (HDL) and low-density liquid (LDL) in liquid water.

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