Uniqueness of water compared with other liquids under nano-confinement

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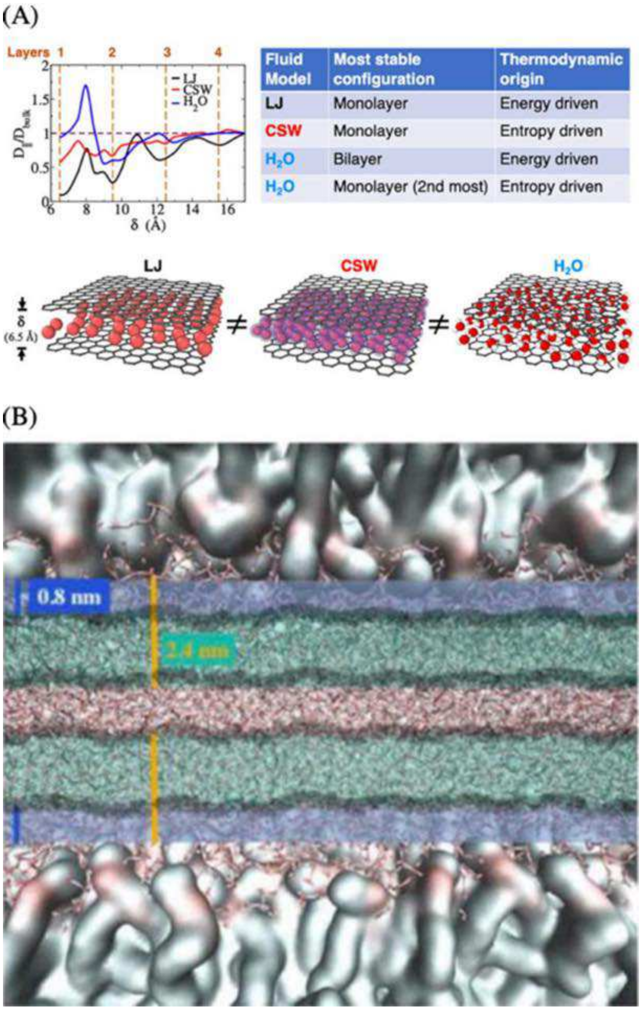

Fig. 1. (A) Comparison of the diffusion of a normal fluid (LJ), an anomalous fluid (CSW), and water in a graphene nanopore. Their free energies change differently with the pore size (upper right table), and water is the only one that diffuses faster than bulk under sub-nm confinement (upper left panel). (B) Atomistic simulations of water between two membrane leaflets, Martelli et al. (2021). Away from the lipids (smooth surfaces), we schematically mark three regions: lipid-bound water (blue), unbound water (green), bulk water (red and withe stick molecules), and the interfaces between them (dark regions). Water penetrates between the lipids and persists there even at low hydration.

Living organisms, viruses, and technological devices have water layers between their cells or parts and can die or stop working when dehydrated. But why water and not any other fluid? What makes water unique when it is in these tiny pores? We investigate why the water in a pore tinier than one-millionth of a hair moves faster than free water, while other fluids do not. We show that it all depends on the peculiar hydrogen bond interaction of water [1] (Fig. 1A). The results might be a key factor contributing to the solution of the United Nations Sustainable Development Goals about clean water and sanitation and relate to the switching behavior observed in a hydrated graphene nano-memristor proposed as a memory device that could store the data of 100 trillion flash memories in just 1 cm^3 for quantum computing [2, 3].

On the other hand, water's uniqueness is also essential in cellular membranes. We revise and extend the concept of 'hydration' or 'biological water', i.e., the nanoscopic layer of water covering the surface of biosystems. We find and discuss the existence of a bound/unbound water interface and its effect on dynamics and structure as far as 2.4 nm away from the membrane (Fig. 1B). The results might be relevant for understanding the role of water in biological activity, e.g., the efficacy of new drugs or vaccines [4, 5, 6].

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