New 'Tunneling' State Of Water Molecules Is A Rulebreaker

Physicists at the Oak Ridge National Laboratory identified a new water state that breaks the fundamental rules of water. The "tunneling" state allows molecules, when in confined spaces, to scatter around and pass through potential walls. (Jeff Scovil | Oak Ridge National Library)

Under extreme confinement, water molecules undergo a "tunneling" state breaking the rules of known fundamentals seen in gas, liquid, or solid state, a new study has found.

Scientists at the Department of Energy's Oak Ridge National Laboratory (ORNL) used neutron scattering and computational modeling to reveal a new water molecule state. The water molecule tunneling was observed while restricted in a mineral beryl with hexagonal ultra-small channels that measures only 5 angstrom across. Past studies have suggested atomic hydrogen also undergo tunneling in other systems, but unlike what was observed in the present research.

An earlier experiment, using molecular simulation and computational algorithm, also revealed a new frozen-water state in clathrate configuration wherein water molecules interlock and form a cage-like foundation.

The experiment conducted at ORNL's Spallation Neutron Source in collaboration with the Rutherford Appleton Laboratory in the United Kingdom revealed that while in the tunneling state, the molecules of water become scattered around a ring allowing it to take up a double top-like shape.
The discovery, according to the researchers, describes the behavior of water molecules present in tightly confined areas such as cell walls, soils, and rocks.

Alexander Kolesnikov, lead author from the laboratory's Chemical and Engineering Materials Division, said that the water molecules show quantum motion as it passes the potential walls -- something that is not seen yet in conventional models.

"This means that the oxygen and hydrogen atoms of the water molecule are 'delocalized' and therefore simultaneously present in all six symmetrically equivalent positions in the channel at the same time," said Kolesnikov. "It's one of those phenomena that only occur in quantum mechanics and has no parallel in our everyday experience."

Kolesnikov added that the average kinetic energy of the protons in the water was taken at its zero temperature. It is also notable that the energy is 30 percent less while it is in solid water or bulk liquid -- a behavior that breaks the rules of the accepted models grounded on energies of its vibrational modes.

ORNL's senior research scientist and co-author Lawrence Anovitz believes that their discovery challenges the fundamental understanding about water.

The new finding has many important uses in the real world. Thermodynamic properties and water behavior, while in extremely restricted locations, such as cell membrane channels in carbon nanotubes and mineral interfaces in a range of geological environments can be easily understood using the tunneling state of water.