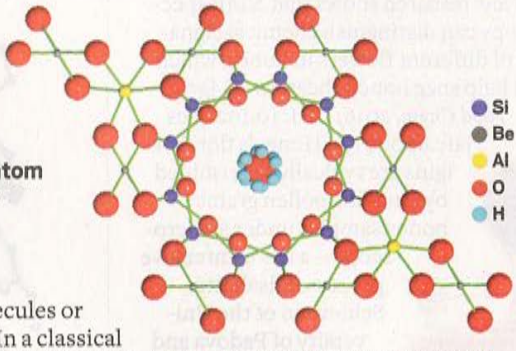
CHEMICAL BONDING

Delocalized form of water identified

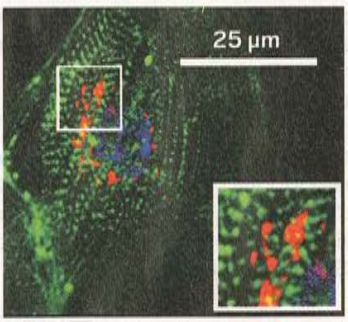
A multidisciplinary research team has found that a solitary, confined water molecule can exist in a previously unidentified state in which protons and electrons form a delocalized ring around the oxygen atom (*Phys. Rev. Lett.* 2016, DOI: 10.1103/physrevlett.116.167802). Alexander I. Kolesnikov of Oak Ridge National Laboratory and coworkers used neutron scattering to study water molecules trapped in cavities of the mineral beryl. These crystal lattice cavities are just large enough to fit one water molecule, with no hydrogen



A water molecule trapped in a beryl crystal cavity takes on multiple simultaneous orientations—it appears to have a central oxygen atom surrounded by an array of hydrogen atoms.

bonds to other water molecules or to the beryl cavity atoms. In a classical view, the water molecule sits with the oxygen atom roughly in the center of the cavity and its two hydrogens pointing toward one of the faces, held in place by an energy barrier to rotation. Taking a quantum mechanical view, the researchers found that the water molecule can "tunnel" through the barrier and exist in multiple orientations simultaneously. The resulting structure has the centrally located oxygen surrounded by concentric rings of delocalized electrons and protons. The symmetry of this form means that the water molecule has zero electric dipole moment. The team suggests this newfound state of water could also occur in other confined spaces, such as cell membranes.—JYLLIAN KEMSLEY

goal, this type of cellular manipulation could give surgeons a source of tissue to help repair damage after a heart attack. A team led by Sheng Ding of the University of California, San Francisco, developed the method and has shown that the new cardiomyocytes, which are muscle cells that help the heart beat, can repair cardiac damage in mice (*Science* 2016, DOI: 10.1126/science.aaf1502). Researchers have been



This immunofluorescence image shows chemical markers identifying a fibroblast that has been converted to a cardiac-like cell. The inset shows areas at higher magnification.

group selected 83 compounds, which included enzyme inhibitors and epigenetic modulators known to help reprogram cell growth and development, to steer the cells toward cardiac function. The researchers exposed human foreskin fibroblasts to various combinations of the compounds, finding that one set of nine compounds accomplished the conversion to cardiac-like cells with beating behavior. They