



the simulation was performed with the cell parameters found experimentally when pressure was fully released.

“At first, we hadn’t checked the material to see if it had remained the same at ambient pressure,” Tabacchi says. But the experimentalists quickly confirmed that the ethanol dimers and water tetramers were still in place in the zeolite channels at ambient pressure. This validated the discovery. “We had taken a disordered liquid solution and converted it into a new material—a solid with a normal distribution of water and ethanol,” Tabacchi says.

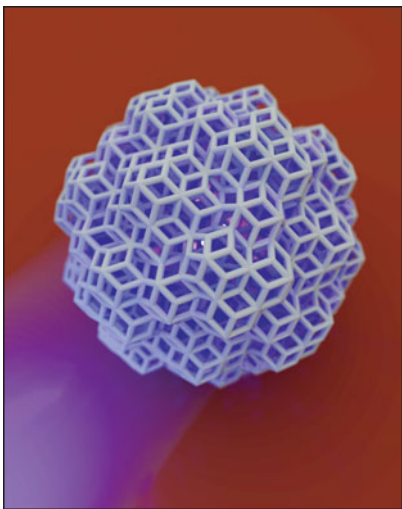
The researchers theorize that perhaps the high pressure causes some slight modification of the structure that makes the material stable at ambient pressure as well. Separating ethanol from water is a key issue in biofuel production, so this zeolite might have a practical application. Tabacchi envisions trying more complex systems with a different zeolite to accommodate molecules of larger size, like the chromophores of a dye, to create a material featuring a 2D arrangement of photoactive molecules that perhaps can capture solar energy more efficiently than is now possible.

“Beautiful and fascinating” is how Gion Calzaferri, a professor in the Department of Chemistry and Biochemistry at the University of Bern, Switzerland, who was not involved in this research, describes the work. “The discovery of this host–guest composite allows us to dream about materials having fascinating physical (and perhaps also chemical) properties we have not seen so far. It may be the beginning of a new area of research exploring one-dimensional nanomaterials based on two different parallel running molecular wires.”

Tim Palucka

Finite-difference methods used to model photonic wave localization in 3D quasicrystals

Scientists at the Korea Institute of Science and Technology (KIST), led by Kayhun Hur, have made the first theoretical demonstration of the localization of photonic waves in a three-dimensional (3D) quasicrystal. This promising finding suggests that quasicrystals could one day be precisely engineered to control localization of electrons, phonons, and photons.



Schematic representation of photonic wave localization in a three-dimensional icosahedral quasicrystal. Incident photonic waves are trapped in the quasicrystal due to localization. Image courtesy of Kahyun Hur, Korea Institute of Science and Technology.

Quasicrystals are a unique type of crystalline material with local order but no long-range periodicity. The discovery of these materials in aluminum-manganese alloys garnered materials scientist Dan Shechtman the 2011 Nobel Prize in Chemistry. Quasicrystals exhibit unusual properties due to their mixed structural characteristics. Because translational symmetry strongly governs the transport properties of every form of wave, wave transport in quasicrystals—including localization—has been a long-standing area of research interest. In particular, icosahedral quasicrystals possess a 3D photonic bandgap, which could allow for control of light at the nanoscale.

In crystalline materials, waves with wavelengths commensurate with the crystal’s periodicity can transmit without scattering loss, leading to ballistic transmission. In contrast, because of frequent scattering, wave transport in disordered materials is usually described by random walks, resulting in diffusive transmission. Quasicrystals exhibit both diffusive transport due to their aperiodicity, along with a well-defined coherent path due to their crystalline nature. These materials therefore provide a compelling test system to investigate wave localization in three dimensions.

As reported in a recent issue of *Nature Physics* (doi:10.1038/NPHYS4002), the KIST team used finite-difference methods to model photonic wave localization in a 3D icosahedral quasicrystal. Wave localization phenomena were investigated by

analyzing the spatial and temporal evolution of photonic waves. Using photonic band structures of quasicrystals called rhombic triacontahedrons (see Figure), the research team generated transmission spectra and compared these to a diamond structure for reference. Their findings demonstrate that wave localization occurs in quasicrystalline materials. This fundamental insight will help researchers to determine how to control or steer waves in quasicrystals.

“This proof-of-principle study breaks new ground by showing that it is possible to localize photonic waves even in a disorder-free medium solely relying on the absence of translational invariance in quasicrystals,” says Bohm-Jung Yang of Seoul National University in South Korea, who was not involved in the research.

Hur and colleagues suggest that wave localization in quasicrystals can be utilized for a variety of applications related to wave transport: replacing reflecting mirrors in lasers, incorporating quasicrystalline nanostructures into thermoelectrics as phononic insulators to improve the thermoelectric figure of merit, or as acoustic insulators. In addition, the superior wave trapping properties of quasicrystals make them excellent candidates as light-trapping layers in photovoltaics.

“Due to the universal features of wave transport in 3D quasicrystals, we believe there will be other, huge potential applications of these materials based on control of wave localization,” Hur says.

Aditi Risbud