AI
No Longer Science Fiction
MAKING LIGHT WORK OF COMPUTING

If you can make a single photon, tell it how to spin and tell it where to go, you have a basic element for next-generation computers that work with light instead of wires.

Atom-thick materials make this possible, as demonstrated by several labs. Rice University engineers have developed an understanding of the mechanism by which two-dimensional materials can be manipulated to produce the desired photons.

The lab of materials theorist Boris Yakobson reports that by adding pre-arranged imperfections to atom-thick materials like molybdenum disulfide, they become capable of emitting single photons in left or right polarization on demand.

The discovery through first-principle simulations was detailed in the American Chemical Society journal Nano Letters. The photons come from designer defects in the 2D lattice that add their own peculiar electronic properties to semiconducting materials. In the case of molybdenum disulfide, a dash of rhenium in the right spot makes a configuration of atoms with energy states that sit comfortably inside and are isolated from the material's natural band gap.

Once in place, the magnetic moments of atoms in the defect can be aligned with a polarized magnet. Exciting them with light brings them to a higher energetic state, but the band gap is large enough that the energy has only one way to go: out, as a coveted single photon.

The defect creates a two-level energy state isolated from the semiconducting material's natural band gap. Illustrations by Sunny Gupta.
Defects in exotic, two-dimensional materials known as transition-metal dichalcogenides may be just what scientists need to advance quantum computing. Theoretical models by scientists at Rice University have predicted how particular 2D materials could be modified to produce photons with custom polarization.

“Atoms that make up the defect have magnetic moments that can be random, but a magnetic field can bring them to a particular quantum state, either up or down,” Yakobson said. “After that, if you shine light on the defect, it goes from its ground state to an excited state and emits a desirable single photon, with specific polarization. That makes it a bit, which will be useful in quantum information processing.”

“The defect’s optical transition lies in the optical fiber telecommunication band, which is ideal for integration into photonic circuits,” added Rice graduate student and lead author Sunny Gupta.

All of the 2D candidates modeled by Yakobson, Gupta and alumnus Ji-Hui Yang are dichalcogenides, semiconductors that incorporate transition metals and chalcogens.

They also modeled tungsten diselenide, zirconium disulfide, boron nitride, tungsten disulfide, diamine (2D diamond, which labs are beginning to synthesize) and, for comparison, 3D diamond.

“One of the advantages we argue here relative to 3D materials is that extraction of the photon is much easier, because the material is basically transparent and there is so little thickness,” Yakobson said. “Photons are not so easy to extract from 3D materials, because they may get stopped by internal reflections, or be refracted, or just dissipate in the material. But 2D materials are more open and the photon is produced near the surface, making its extraction for utility easier.”

“The defect’s optical transition lies in the optical fiber telecommunication band, which is ideal for integration into photonic circuits.”

—Sunny Gupta
Graduate Student, Materials Science and Nanoengineering