The shape of things to come for quantum materials?

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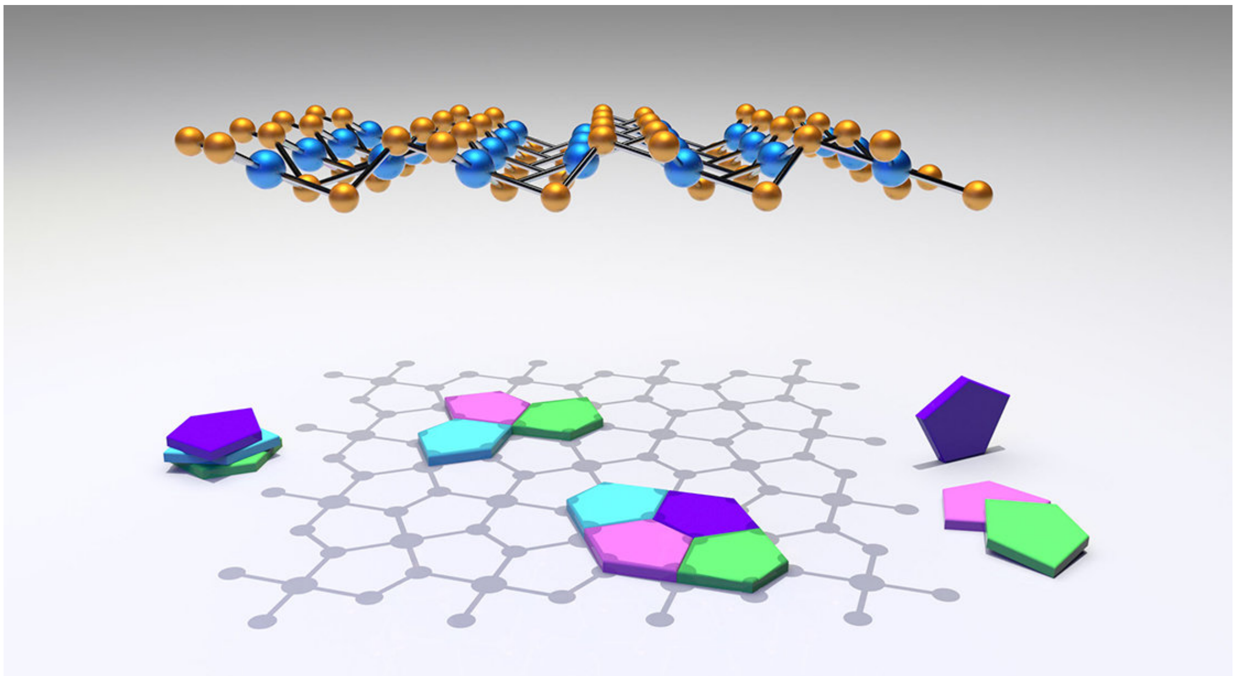

Theory predicted the existence of materials composed of pentagonal “tiles” (purple, teal, green, and pink). Now, researchers have proven these materials exist. Scientists made and characterized the first-ever sheets composed of pentagons of palladium diselenide. Rather than being flat, the material is puckered. The top image shows this puckered structure with blue palladium atoms and gold selenium atoms. The puckered structure leads to interesting electronic properties. These tiles are promising building blocks for air-stable electronics, photonics, and other technologies. Credit: US Department of Energy

For the first time, researchers isolated and characterized atomically thin 2-D crystals of pentagons bonded together in palladium diselenide (PdSe2). The research confirmed predictions that the puckered structure would be stable.

The unique structure of the material results in beneficial properties. It has fast-moving electrons. Also, it is stable in air. Other 2-D semiconductors are not stable in air. These properties may enable advanced uses in detectors, solar cells, and transistors. Further, this material could advance superconductivity for electrical flow without losses, piezoelectric sensors, and energy-efficient computing.

Most 2-D crystals studied to date are a lattice of hexagons—for example, graphene, transition metal dichalcogenides, and black phosphorus—and the lattice layers may be planar or puckered. Theory predicted a family of 2-D crystalline materials with lattices made of pentagonal "tiles." Sheets of pentagons are unusual even in nature. Now, a team led by Oak Ridge National Laboratory has proven experimentally the existence of one member of this family. The researchers used bulk crystals made by a group from Nanyang Technological University; they exfoliated the crystals to obtain puckered layers of PdSe2. Using high-resolution scanning transmission electron microscopy, they characterized layers having different thicknesses. Micro-absorption optical spectroscopy, Raman spectroscopy, and first-principles calculations showed layer thickness changed the band gap. The band gap is the energy range in a solid at which electronic states cannot exist. The thickness changed the band gap from 0 in the bulk (multiple layers) to 1.3 electron volts in single monolayers. That finding paves the way for pentagonal 2-D materials with tunable band gaps, which may bring new capabilities to electronics and photonics. Most 2-D materials have highly symmetric lattices and, as a result, exhibit isotropic behavior—that is, a physical property has the same value when measured in different directions. In contrast, pentagonal 2-D PdSe2 is anisotropic—meaning property values differ when measured in different directions. Pentagonal 2-D materials may allow a new degree of freedom for designing conceptually new optoelectronic and electronic devices not possible using other 2-D materials. Moreover, the material is stable in air, which is not true of many other 2-D semiconductors. For example, it is less susceptible to oxidation than black phosphorus, another promising 2-D material with a tunable band gap. The discovery of additional puckered pentagonal building blocks may advance applications in low-energy optoelectronics, piezoelectrics, thermoelectrics, and spintronics.

More information: Akinola D. Oyedele et al. PdSe2: Pentagonal Two-Dimensional Layers with High Air Stability for Electronics, *Journal of the American Chemical Society* (2017). DOI: 10.1021/jacs.7b04865

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