

Unusual rods get thicker when stretched

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Day-to-day experience teaches us that stretching an object makes it thinner; pushing it together makes it thicker. However, there are also materials that behave contrary to our expectations: they get thicker when stretched and thinner when compressed.

Known as "auxetic" substances, these materials include some foams and special crystals. Researchers at the Bar-Ilan University and the Israel Institute of Technology have now used quantum mechanical calculations to identify the first class of chemical compounds that behave auxetically on a molecular level.

When a usual material is, for example, hit by a ball, the material "flows" outward from the impact zone making the point of impact weaker. However, in auxetic materials, the matter "flows" inward, thus strengthening this zone. Such materials would be advantageous for bulletproof vests. Auxetic materials also provide interesting possibilities for medical technology. The introduction of implants such as stents to hold open blood vessels would be easier if, under pressure, the device would get thinner instead of thicker in the perpendicular direction.

In the auxetic materials known to date, the unusual behavior is a macroscopic property that stems from a special arrangement of the particles within the material, such as a particular weblike structure. Nanoscale auxetic materials are so far unknown.

By using quantum mechanical calculations, a team led by Shmaryahu Hoz has now predicted that there also exist certain molecules that behave

auxetically: a class of compounds known as polyprismanes. These are rod-shaped molecules built up of several three-, four-, five-, or six-membered rings of carbon atoms stacked on top of each other. The prismanes made of three- and four-membered carbon rings show roughly equal auxetic effects, regardless of the number of stacked rings. The ones made of five- and six-membered carbon rings demonstrate significantly higher auxetic effects. Of all of the variations for which calculations were carried out, the prismane made of four six-membered rings showed the strongest effect. The researchers have not yet been able to unambiguously explain why prismane molecules behave auxetically.

"Although prismanes were discovered over 30 years ago, very few representatives of this class of compounds have been synthesized so far," says Hoz. "We hope that our insights will act as an incentive to produce and characterize more prismanes."

Citation: Shmaryahu Hoz et al., Auxetics at the Molecular Level: A Negative Poisson's Ratio in Molecular Rods, *Angewandte Chemie International Edition* 2006, vol. 45, No. 36, doi: 10.1002/anie.200601764

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