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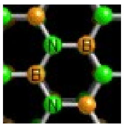

Inelastic boron nitride

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Rubio, lifting the hex on BN

The results of inelastic X-ray scattering and other techniques have been combined with *ab initio* calculations to characterise and explain the behaviour of the superficially simple binary material boron nitride. Insights from the research carried out by Ángel Rubio of the University of the Basque Country and colleagues there and at the European Theoretical Spectroscopy Facility could lead to new ways to exploit the electronic and mechanical properties of hexagonal boron nitride.

Boron nitride is currently used as a coating material for reactors and as an insulating material. However, its intriguing electronic properties, which include high resistance, and blue light emission making it a potentially useful material for the development of optoelectronics in optical data storage media and as high resolution lasers as well as in aerials.

Of particular interest from the materials scientists' perspective, is the revelation that macroscopic structures in boron nitride emerges from nanostructured molecular solids through weak, van der Waals type interactions. The researchers had demonstrated previously that van der Waals interactions play a critical role in the stability of these boron nitride nanostructures. On the other hand, they are also key to the absorption and emission properties that occur in the blue and near ultraviolet region of the spectrum.

Also of interest from the developmental point of view as well as understanding related materials is that boron nitride is isoelectronic with elemental carbon and so can exist as isomorphic forms equivalent to diamond, graphite, and even the spherical and tubular fullerenes. Specifically, hexagonal boron nitride is analogous to graphite, but whereas graphite is electrically conductive, hexagonal BN is an insulator. Moreover, it is a high bandgap semiconductor.

"Experimental data and calculations show an outstanding agreement," say the researchers. Interestingly, the work also "reconciles the controversies raised by recent experimental data obtained by electron-energy loss spectroscopy and second-order Raman scattering." Rubio told SpectroscopyNOW that, "One major finding is that the band-gap is independent of size and dimensionality (whether we have 3D hexagonal BN, a sheet or a nanotube) and that this gap can be tuned."

Rubio received the 2006 DuPont Science Award for his work on theoretical nanoscience and molecular nanotechnology and undertook the current research with colleagues Jorge Serrano and Alexei Bosak, and Michael Krisch at the European Synchrotron Radiation Facility, in Grenoble, France, Raul Arenal of the Argonne National Laboratory, Illinois, Kenji Watanabe, Takashi Taniguchi, and Hisao Kanda of the National Institute for Materials Science, in Tsukuba, Japan, and Ludger Wirtz of the IEMN (CNRS-UMR 8520), in Villeneuve d'Ascq, France.

Related links:

- **Phys Rev Lett 2007, 98, 095503**
- **Rubio Page**
- **DuPont Prize**
- **Boron Nitride**

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