New possibilities for boron nanotubes

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Even though some scientists have managed to grow boron nanotubes, the nature of their structure is unknown. Different theories have been proposed regarding boron nanotube make-up, but they often result in structures that are not optimally stable.

Sohrab Ismail-Beigi, a professor at Yale University, and his graduate student Hui Tang, believe they have found the most stable structure to date. Their theory is based upon something that scientists have overlooked in the past: the importance of the difference between two-center and three-center bonding.

“Appreciating these two different bonding schemes explains why the new structures we have found are more stable, and also teaches us more about other possible boron structures yet to be considered,” Ismail-Beigi tells *PhysOrg.com*.

“For carbon nanotubes,” he points out, “the graphene structure based on two-center bonding is most stable. This is not the case for boron. We are talking about an entire new class of boron sheets, with new sets of possible structures, that are more stable than previously assumed.” Ismail-Beigi and Tang’s theory of boron nanotube bonding is published in a *Physical Review Letters* piece titled “Novel Precursors for Boron Nanotubes: The Competition of Two-Center and Three-Center Bonding in Boron Sheets.”

Instead of two-center bonding, in which two atoms share two electrons in a bond, an essential feature of boron is its tendency to three-center

bonding, in which “electrons are shared among three atoms simultaneously.” Ismail-Beigi continues: “We really thought about it and realized that three-center bonding makes the new class of boron structures more stable.”

When this theory is applied, Ismail-Beigi hopes that it leads to the development of boron nanotubes that can act as conductors in a way that carbon nanotubes can’t. “Graphene, which is used for carbon nanotubes, is a two-dimensional system and not a true metal,” he explains. “With carbon, you take the 2-D graphene and roll it up to make a nanotube. Depending on the precise details of the rolling, you can end up with the fact that of all the tubes of the same diameter, you get conductors only about one-third of the time. And they aren’t very good conductors.”

Ismail-Beigi says that boron nanotubes would make better conductors. “It’s a metal, and it’s a matter of robustness.” He goes on to point out that in boron nanotubes, the spiral pattern in rolling (called chirality) would not be as much of a hindrance to conductivity. “In these conductors of the same diameter, chirality would still matter, but all of the boron nanotubes would still be decently conducting.”

The properties that Ismail-Beigi expects would result in boron nanotubes would make them candidates to replace carbon nanotubes in some cases. Metallic systems for one-dimensional electronics could be made better with boron, and it is possible that boron nanotubes would possess higher super-conducting temperatures than carbon nanotubes. “If we’re looking for better conducting nanotubes,” he insists, “it makes sense to start moving away from carbon nanotubes.”

The first step in moving away from carbon, Ismail-Beigi says, is understanding the structure of boron nanotubes. “We’re trying to see what is a likely structure for boron, and once you know that, you can determine its properties and find uses.” Nailing down the three-center

bonding, and proposing sheets with hexagonal and triangular motifs is one way to understand the structure of boron nanotubes, leading to further theories about how boron may act.

“One of the preliminary things that we find is that it seems as though boron nanotubes might change from metals to semiconductors under pressure,” explains Ismail-Beigi. He points out that this is just one of the interesting mechanical properties that might be seen in boron nanotubes. Ismail-Beigi also mentions that the boron structures they have found have conductivity only in the pi-manifold (made from atomic p states). “It is interesting that the electronic conductivity happens in the out-of-plane [pi] states and not the other in-plane ones.”

“This entire field is very new,” he continues. “We’ve only just finally figured out where the atoms are, and now we can say what some of the properties might be.”