Carbon nanostructures at the forefront: nanotubes, graphene, and beyond

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Significant advances in Materials Science have been achieved by harnessing specific functionalities of nanostructures, such as improved mechanical, electrical and thermal properties, for particular applications. Predictive *ab initio* calculations suggest that designer nanostructures, including diamond nanowires inside nanotubes [1] or carbon foam nanostructures [2], shown in Fig. 1, should display unique electronic, mechanical and thermal properties. Twisted carbon nanotube ropes [3] may store reversibly much more energy than other energy storage devices [4]. Unusual thermal conductivity can be expected in graphitic nanostructures including graphene, nanotubes and schwarzites. Successful synthesis of such nanostructures precludes detailed understanding of their microscopic formation mechanism. Since direct observation of such atomic-scale processes is very hard by experimental means, computer simulations are a welcome alternative to gain microscopic insight into the underlying processes.

[1] Jinying Zhang, Zhen Zhu, Yanguan Feng, Hitoshi Ishiwata, Yasumitsu Miyata, Ryo Kitaura, Jeremy E. P. Dahl, Robert M. K. Carlson, Natalie A. Fokina, Peter R. Schreiner, David Tománek, and Hisanori Shinohara, Angew. Chem. Int. Ed. **52**, 3717 (2013).

[2] Z. Zhu and D. Tomanek, Phys. Rev. Lett. **109**, 135501 (2012).

[3] David Teich, Gotthard Seifert, Sumio Iijima, and David Tomanek, Phys. Rev. Lett. **108**, 235501 (2012).

[4] David Teich, Zacharias G. Fthenakis, Gotthard Seifert, and David Tománek, Phys. Rev. Lett. **109**, 255501 (2012).

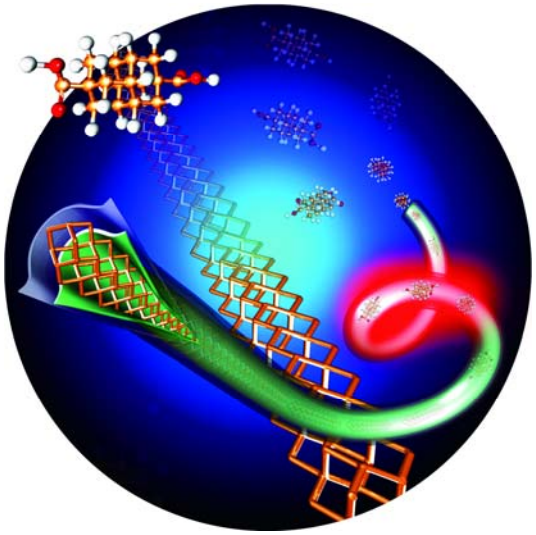

Figure 1
Formation of a diamond nanowire inside a nanotube (cover page of Angew. Chem. Int. Ed., Vol. **53**, issue 13, March 2013).