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Twisting Graphene into Carbon Nanotubes[1] OLEG O. KIT, University of Jyvaskyla, Finland, TUOMAS TALLINEN, L. MAHADEVAN, Harvard University, JUSSI TIMONEN, PEKKA KOSKINEN, University of Jyvaskyla, Finland — Carbon nanotubes are usually described as being rolled up from graphene sheets; this process, however, have never been realized experimentally. We showed that graphene can indeed be transformed into nanotube by twisting [1]. Further, we showed that tube formation can be well-explained within classical theory of elasticity—in fact the very mechanism of tube formation can be observed by twisting a strap from one's backpack (try now!). Furthermore, we showed that nanotube chirality may not only be predicted, but can also be controlled externally. The quantum molecular dynamic simulations at T=300K were achieved thanks to the revised periodic boundary conditions (RPBC) approach [2-3]. The structures similar to simulated have been recently observed experimentally [4]. This novel rote for nanotube formation opens new opportunities in nanomaterial manipulation not restricted to carbon alone. In the presentation, I will describe tube formation, as well as outline the easy and efficient technique for distorted nanostructures simulation, the RPBC approach.

[1] O. O. Kit et al. arXiv:1108.0048
[2] P. Koskinen & O. O. Kit PRL 105, 106401 (2010)
[3] O. O. Kit, L. Pastewka, P. Koskinen PRB 84, 155431 (2011)
[4] A. Chuvilin et al. Nature Materials 10, 687 (2011)

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[X] Prefer Oral Session
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