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First principles **study of Crystalline Bundles of Single-Walled Boron Nanotubes**[1] KAH CHUN LAU, ROBERTO ORLANDO[2], RAVINDRA PANDEY, Department of Physics, Michigan Technological University, Houghton, MI — *First principles* calculations based on density functional theory are performed to study the structural and electronic properties of the crystalline bundles of (n,0) zigzag-type single-walled boron nanotubes (SWBNT). The results predict a substantial modification in the properties of SWBNT bundles relative to those of the isolated nanotubes. The predicted modification can be attributed to a significant interplay between intra- and inter-tubular bonds in determining the stability of SWBNT bundles, analogous to the role played by intra- and inter-icosahedral bonds in the boron crystalline solids. The result shows the SWBNTs exhibit polymorphism, which is likely to be the cause of the difficulty in growing SWBNTs experimentally.

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[2]Permanent Address: Dipartimento di Scienze e Tecnologie Avanzate, Università del Piemonte Orientale, Via Bellini 25/G, 15100 Alessandria, Italy

Kah Chun Lau
Department of Physics, Michigan Technological University, Houghton, MI

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