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Straddling to staggered band gap transition and optics of double-walled carbon nanotubes ALEX KUTANA, VASILII I. ARTYUKHOV, BORIS I. YAKOBSON, Department of Materials Science and NanoEngineering, Rice University, Houston, TX — Single-walled carbon nanotubes have outstanding optical properties that show pronounced dependence on their helicity. Techniques for helicity separation or selective growth enabled extensive studies of their optics. However, in double-walled nanotubes (DWNT) the inner wall helicity is hard to control. Only recently effective techniques for DWNT sorting and helicity assignment were developed,[1] and experiments on helicity-controlled DWNT reveal remarkable new optical effects.[2] Here we study the effect of breaking of π band symmetry by wall curvature, creating a potential difference between the inside and outside of a nanotube. In DWNT, this intrinsic flexoelectric voltage, $V \propto 1/R$, shifts the bands of the inner wall, and above a certain threshold the voltage exceeds the band offset ($\propto 1/R^2$), marking the transition from conventional straddling to staggered band structure, where frontier electronic bands are localized on different walls. This has dramatic optical implications which we study using density functional theory and many-body GW+BSE calculations.[3]

[1]A. Loiseau *et al.*, NT14, Los Angeles, CA (2014)
[2]K. Liu *et al.*, *Nat. Phys.* 10, 737 (2014)
[3]V. I. Artyukhov, A. Kutana, B. I. Yakobson, in preparation

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