Abstract Submitted
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Structural dependence of carbon nanotube orbital magnetic susceptibility: tight binding calculations[1] O. N. TORRENS, J. M. KIKKAWA, Department of Physics and Astronomy, University of Pennsylvania — Recent ab initio calculations of the orbital magnetic susceptibility anisotropies in carbon nanotubes (CNTs) have shown large, systematic differences among zigzag CNTs of similar diameters [1]. We theoretically investigate the origin of these trends by applying the zone-folding method within the nearest-neighbor tight-binding approximation to all chiral and achiral semiconducting CNT species with diameters between 0.6 nm and 1.7 nm. Our results show qualitative agreement with the "mod 1" and "mod 2" trends of the ab initio theory and additionally distinguish between trigonal warping and curvature-related effects as physical reasons for the predicted species-dependent spread. Our calculations show (2n+m) patterns similar to those in a recent, experimentally-motivated "fan-out" diagram [2] and can be likewise fit to an analytical four-term chirality expansion. [1] Marques, M. A. L.; d'Avezac, M. & Mauri, F., *Phys. Rev. B,* **2006**, 73, 125433 [2] Torrens, O. N.; Milkie, D. E.; Ban, H. Y.; Zheng, M.; Onoa, G. B.; Gierke, T. D. & Kikkawa, J. M., *J. Am. Chem. Soc.,* **2007**, 129, 252-253

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