Quasi Small-World Nanomaterials : Quantum Studies

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Mississippi State U. — We present results for two studies of quasi-small-world nanomaterials [1,2]. These are materials that would have the connectivity governed by small-world (SW) networks. Hence these materials should have both their critical behavior and transport properties governed by mean-field fixed points, not finite-dimensional fixed points. One study utilizes density-functional-theory to obtain reasonable carbon-based molecules that should have the SW property. In particular, several candidates for quasi-SW nanomaterials (or molecules) based solely on carbon will be presented. Trends in the energy per atom of various types of SW nanomaterials and numbers of carbon atoms will be presented. The transmission coefficient and conductivity for related quantum models of SW nanomaterials connected to metal leads will also be presented. [1] M.A. Novotny, et al, J. Appl. Phys, vol. 97, p.10E510 (2005). [2] M.A. Novotny and S.W. Wheeler, Brazilian J. Phys., vol. 34, p. 395 (2004).

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