

Third Stig Lundqvist Conference on Advancing Frontiers of Condensed Matter Physics:
Fundamental Interactions and Excitations in Confined Systems

“Theoretical Studies of Nanotubes, Nanocrystals, and Some Molecular Systems”

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Abstract

After reviewing some background material on the current status of theoretical investigations of electronic, structural, and other properties of bulk solids, the roles of lower dimensionality and confinement will be addressed. In particular, the extensions of the theory to the nanoscale is of interest to physicists, chemists, biologists, engineers, computer scientists, and others doing basic and applied research on nanoscale systems. Specific examples related to clusters, nanocrystals, fullerenes, and nanotubes will be presented to describe the current status of research in this area and to illustrate the importance of active experimental-theoretical collaborations. The current experimental and theoretical advances on carbon and boron nitride nanotubes will receive the major focus, and some applications will be described.

A Few Background References:

- M. L. Cohen, "Pseudopotentials and total energy calculations," *Physica Scripta* **T1**, 5 (1982).
- M. L. Cohen and J. R. Chelikowsky, *Electronic Structure and Optical Properties of Semiconductors* (Springer-Verlag, Berlin, 1988).
- M. L. Cohen, "The theory of real materials," *Ann. Rev. of Mat. Sci.* **30**, 1 (2000).
- M. L. Cohen, "Quantum alchemy," in *Chemistry for the 21st Century*, edited by E. Keinman and I. Schechter, p. 247 (Wiley-VCH, Weinheim, Germany, 2001).
- M. L. Cohen, "Nanotubes, nanoscience, and nanotechnology," *Mat.Sci. & Eng.* **C15**, 1 (2001).