Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

**Hierarchical Coarse-Grained Models for Polymer Simulations**[1]
SHENG D. CHAO, Institute of Applied Mechanics, National Taiwan University
— Structural and thermodynamic properties of industrial and bioengineering materials can be better investigated using atomistic simulations. However, current large-scale atomistic simulations remain computationally demanding. It is thus desirable to seek alternatives to perform efficient and informative mesoscopic simulations. We have developed a coarse-grained intermolecular force (CGIF) model for polymer nanostructures and nanocomposites. This model can effectively capture the stereochemical response to anisotropic long-range interactions. The coarse-graining procedure forms the basis to perform a hierarchy of simulations starting with the quantum-chemistry calculations to coarse-grained molecular dynamics toward continuum modeling. We have applied this procedure to several cases from alkane to benzene to fullerene. For liquid methane, molecular dynamics simulations using the CGIF model reproduce the structural properties calculated using the atomistic force field. The coarse-grained energetics of benzene clusters has well reproduced the results using electronic structure calculations. The subtle anisotropy in the interaction potential of fullerene dimer is also well represented by the CGIF model and is consistent with that calculated using the Brenner force field.

[1]This work was supported by the National Science Council of Taiwan, ROC.

Sheng D. Chao
Institute of Applied Mechanics, National Taiwan University

Date submitted: 02 Dec 2005 Electronic form version 1.4