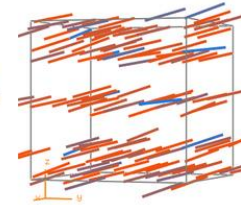


SIMULATION and VISUALIZATION of NANOTUBES and LIQUID CRYSTALS with AViz



JOAN ADLER

COMPUTATIONAL PHYSICS GROUP,
TECHNION-IIT, HAIFA, ISRAEL



TECHNION
Israel Institute of Technology
Department of Physics

COMPUTATIONAL
Physics Group



August 14, 14:00 – 15:00

at room 325 in the third floor of the Engineering building No.6

工学部 6 号館 3 階325号室 (東大本郷キャンパス)

We simulate systems of experimental interest at molecular/atomistic/electronic scale using Simulated Annealing (Metropolis MC), Molecular Dynamics or D(ensity) F(unctional) T(heory) as appropriate or in combination. Original visualization techniques have been developed in our AViz code to enhance understanding of the resulting structures. Two examples will be described: vibrating nanotubes with attached molecules - relevant to their application as N(ano) E(lectro) M(echanical) S(ensors) and liquid crystals containing colloids to enhance conductivity in LCD screens. Background, codes and expository websites will be presented.

Seminar for the group of Professor Nobayasu Ito, University of TOKYO, August, 2017