

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Objective Molecular Dynamics TRAIAN DUMITRICA, Department of Mechanical Engineering, University of Minnesota, RICHARD JAMES, Department of Aerospace Engineering, University of Minnesota — We present a generalization of periodic molecular dynamics that we term *objective molecular dynamics*. It is a method of doing molecular dynamics for a restricted set of atoms, nonperiodically mapping the time-dependent displacements of this small set of atoms onto the full, typically infinite structure, such that the full structure satisfies exactly the full, unconstrained set of equations of molecular dynamics subject to certain group-invariant initial conditions. The method is applicable to a wide variety of interesting molecular structures including the tails, capsids and other parts of many viruses, carbon nanotubes, many of the common proteins, C₆₀ and many other nanostructures now being synthesized, especially via the process of self-assembly. Overall, the strength of the proposed symmetry-based approach is that (i) it heavily reduces the computational effort through a drastic reduction in the number of atoms to be accounted for, (ii) it is compatible with full quantum mechanics, and (iii) the implementation can be done in a general framework, allowing for simulations of a larger class of structures. In addition (iv) the scheme is ideal for obtaining nanomechanical responses since it allows for applying various mechanical deformations. The method is illustrated by simulations of carbon nanotubes.

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Date submitted: 22 Nov 2006

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