Brenner's Code

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Introduction

This document is about Brenner's code. This code can do classical MD simulations. It also has a static mode. It has a fairly complex representation of hydro-carbon potentials, as well as Lennard-Jones potentials. This page is *not* an official page for the code.

The original code can be found here, but I recommend my corrected version as described in section 2. Section 3 has some information about how to run the code with my improvements. The original code comes with README files.

Bug Fixes

I fixed and did not fix various code bugs and code awkwardnesses. A description is here.

Recommended Usage

I made some very basic improvements to the code that I recommend. A description of the changes can be found here

You want to note some key files:

main.f
: The main program. On Unix or Linux, it can now be compiled using the g77 compiler. Do *not* use real*4 precision or some subroutines will have significant round-off errors. The Windows versions already have a ready-to-run program, main.exe, so you do not have to compile on Windows unless you make program changes.

input.d
: Basic program input. A description of this file is here

coord.d
: Starting state of the atoms, as well as their final state. *Note that running the Brenner code overwrites the initial coord.d file with the final state of the atoms after the simulation.* In general, you want to

create a backup of coord.d before running the program. A description of coord.d is here. A starting coord.d file containing a nanotube can be created using the make_tube.f program or, preferably, using the chiral program in the tools available in the installation section. When using make_tube, make sure you have enough "repeat units" to make complete periods. Chiral will ensure complete periods automatically.

parameters.inc

Sets the available storage. May need to be changed for large computations. Also, when using tight binding, NATX will need to be set to the actual number of atoms. After changing this file, main.f must be recompiled.

param_mod.f

Changes various program options.

After changing any .f or .inc file, main.f will have to be recompiled.

Tools

This is a set of separate programs, not part of the Brenner code, that can produce and manipulate coord.d-type files, including single and multi-wall nanotubes. More information is here.

Advanced Information

For more advanced use of the Brenner program, documentation about it can be found here.

Installation

To get the program fixes, basic improvements, and separate tools, select *one* of the following:

- Unix or Linux: click here.
- Windows, using g77: click here.
- Windows, using the Watcom IDE: click here.

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