1. **Description**

This is a systematically coarse-grained polystyrene system. One bead in this system represents one polystyrene monomer. To precisely reproduce the properties of polystyrene, monomers is coarse-grained to two types, one is R and the other is S.



Radius of gyration, bond distribution, angle distribution, and radial distribution function obtained from this system is in good agreement with atomistic MD simulations. The calculated structures in CG simulations by GALAMOST can be compared with that in AA simulations. The benchmark results are given as follows or can be seen in “Tao Chen, Hu-Jun Qian, You-Liang Zhu, and Zhong-Yuan Lu, Structure and Dynamics Properties at Interphase Region in the Composite of Polystyrene and Cross-Linked Polystyrene Soft Nanoparticle, Macromolecules 2015, 48, 2751−2760”.





1. **System**

The chain length of polystyrene is 100, temperature is 500K, pressure is atmospheric pressure and time step is 5 fs (in GALAMOST script, this parameters are represented by reduce unit). The input potential data (in table.dat) which can be obtained by IBI or IMC are in the form of C0, C1, C2, and C3 for a cubic spline function.

1. **Commands**
2. Run the simulation by:

chmod +x galajob.gala

./ galajob.gala --gpu=0 >a.log&

1. The bond length distribution, angle distribution, and radial distribution function can be analyzed by the GALAMOST Plug-Ins “galaTackle” by the commands:

/opt/galamost3/galaTackle filename.xml

Then, select the functions by index and enter, such as the options: 3 RDF, 4 bond\_distri, and 5 angle\_distri and enter. It should be noted that the R monomer is represented by “1” and the S monomer is represented by “2” in this simulation.

1. The PBC conditions can be removed by:

/opt/galamost3/galaTackle filename.xml; select the function of 9 and enter; a new “filename. reimage.xml” will be generated.

And then see the processed configuration by:

vmd –hoomd filename. reimage.xml