

This paper presents a coarse-grained model for PET, using a new method to obtain the nonbonded coarse-grained potentials. This method does not require iteration and may provide more precise potential functions. The coarse-grained force field is used to study various molecular weights, and the scaling exponents for end-to-end distance, radius of gyration and self-diffusivity are reported. An entanglement analysis is also provided.

The paper is interesting, relevant and well written. I recommend that it be accepted in its current form. The comments below are either trivial or up to the authors to implement.

1. on page 3, the authors list polymers for which coarse-grained models are available. I've also seen models for polyethylene, polyethylene oxide, and polyisoprene, if the authors wish to have a complete listing.
2. The A beads in Figure 1 are very dark [un-seeable, really] when the paper is printed in black and white.
3. Top of page 11, Figure 3 is referred to when I think the authors meant Figure 4.
4. The AA, AB, BB pair distribution functions look almost identical whereas the CG potentials for AA, AB and BB are quite different. This must result due to differing influence of “more than pairwise” interactions. It may be interesting to explore this further.
5. I wonder if different scaling for various dynamic properties could be resolved by first scaling time [single scaling, perhaps using mean squared displacement] and then calculating the various dynamic properties using scaled time coordinates.