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Keffer, David J

From: onbehalfof+lipson-office+macromol.acs.org@manuscriptcentral.com on behalf of lipson-office@macromol.acs.org **Sent:** Wed 10/27/2010 12:42 PM

To: Keffer, David J

Cc: lipson-office@macromol.acs.org

Subject: Macromolecules - ma-2010-02084a

Attachments:

27-Oct-2010

Journal: Macromolecules
Manuscript ID: ma-2010-02084a
Title: "Coarse-grained Molecular Dynamics Simulation of Polyethylene Terephthalate (PET)"
Author(s): Wang, Qifei; Keffer, David; Nicholson, Donald; Thomas, Joshua

Dear Dr. Keffer:

We received a third review we would like you to consider while you prepare your revised manuscript. I have pasted the text of the review below. If you have any questions, please let me know. Thank you.

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Review #3

I liked the work presented in the paper by Wang and at. It is a honest and detailed discussion of a novel coarse-grained model for PET. The authors present a detailed study of the properties emerging from a coarse-grained simulation and compare them to the atomistic simulation. I believe this is a very valuable piece of information for two reasons: 1) the novelty of the system investigated (PET), 2) and the care in the presentation and the extended analysis of the data.

It is disappointing that the Rouse regime for diffusion disappears, however it looks like there is a broad transition to entangled dynamics, which covers the Rouse regime and bridges directly to the short chain scaling exponents. I find this information interesting.

The ballistic regime in the mean-square-displacement should be more extended with respect to the atomistic simulation, and maybe the authors could comment on that as well.

We also suggest a few other comments/changes. The work presented in references 27,28 does not use an “iterative procedure” as stated in page 4 end of first paragraph. Instead given the atomistic description, structural properties and interaction potential are output of the theory. The interaction potential is then used as an input to coarse-grained simulations directly, with no need of an iterative self-consistent procedure (see for example Yatsenko et al. PRL v.93, p.257803 (2004).)

Because the analytical coarse-grained potential is available, a first-principle rescaling of the dynamics can be directly calculated as presented in Lyubimov et al. J. Chem. Phys. v.132, p. 2249031 (2010).

Summarizing, this is a very interesting a carefully done piece of research and the paper should be published in Macromolecules after minor corrections.
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Sincerely,

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