Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY MATERIALS

Coarse-grained force-field for large scale molecular dynamics simulations of polyacrylamide and polyacrylamide-gels based on quantum mechanics

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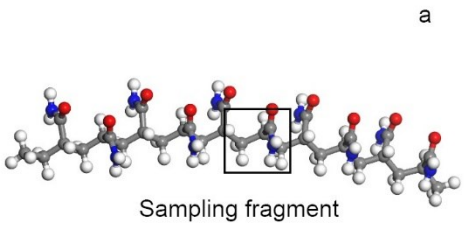
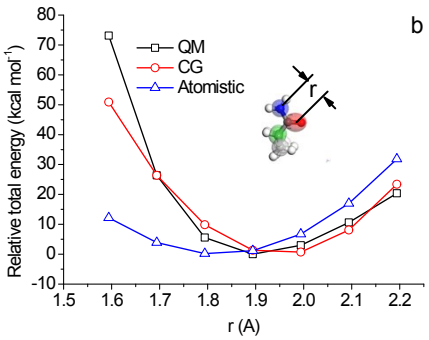
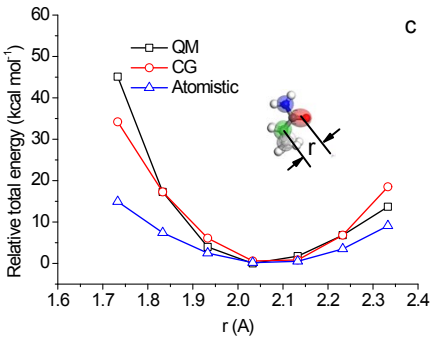
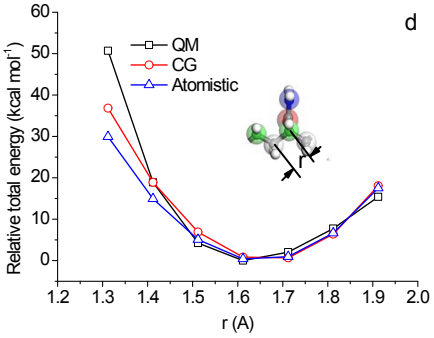
Parameterization of valence interactions of CG-PAM

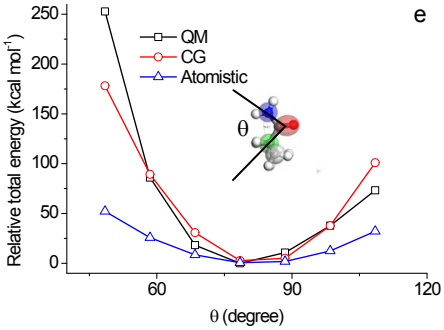
In order to obtain accurate valence interactions, EOS target on a 10-monomer model was calculated using the DFT-PBE-D3 level based on the deformation of a sampling fragment in the chain (**Fig. S1 (a)**). The energy-deformation relationship is shown in (**Fig. S1 (b-g)**). Every EOS is an independent bond-stretching or angle-bending without any changing of other bonds or angels.











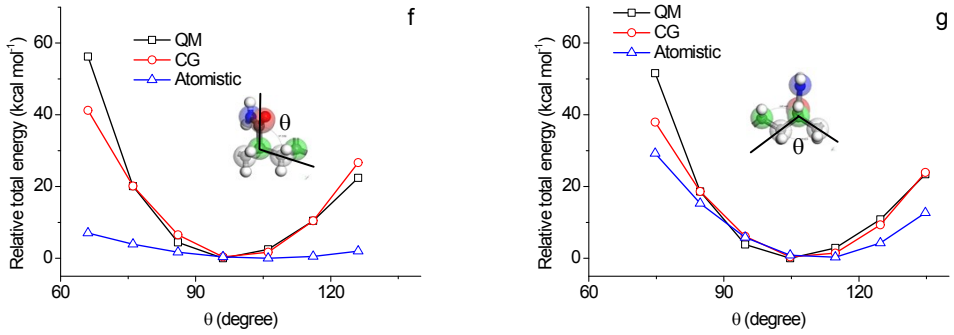


Figure S1 Fragment sampling (a) and the bond-stretching and angle-bending EOS (b-g).

Equilibrium of the CG-PAM system

In the equilibrium of the CG-PAM, the system needs to experience a series of "compress-quench" iterations shown in **Fig. S2**. In each of the iteration step, the compression is performed by directly changing the cell size with a remapping of the particle coordinates at the same scale, while the quenching linearly rises to a top temperature and declines to 300 K. **Fig. S3** shows 800 K is a proper top temperature leading to the lowest final energies and density.

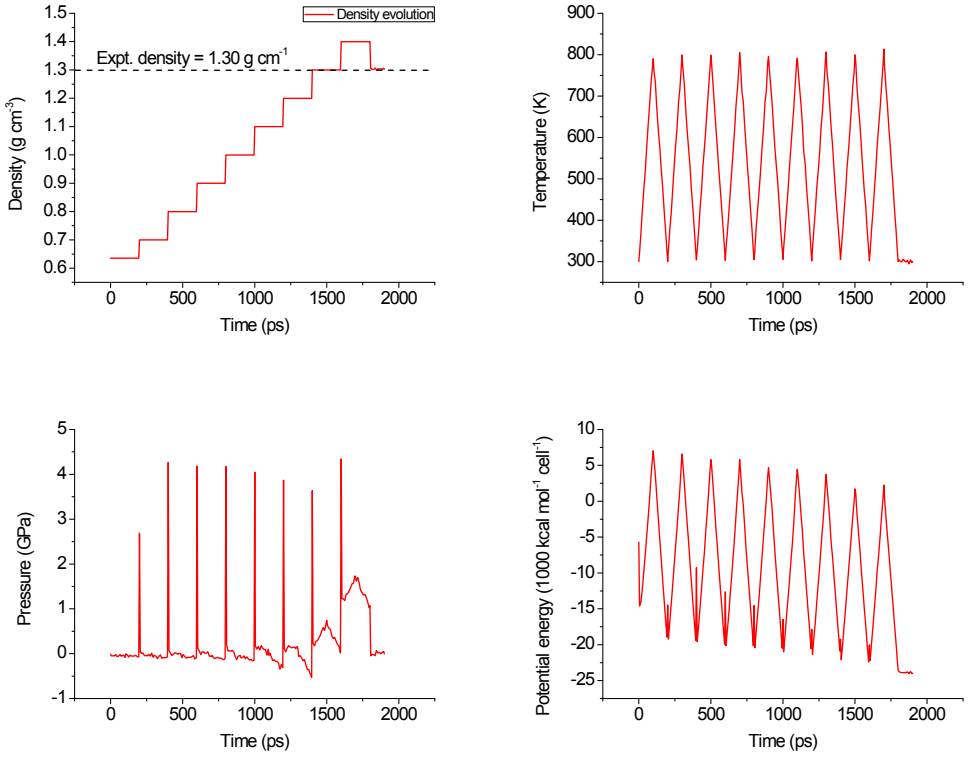


Figure S2 Density, temperature, pressure and potential energy evolution of the equilibrium procedure. Top temperature of the quenching is 800 K.

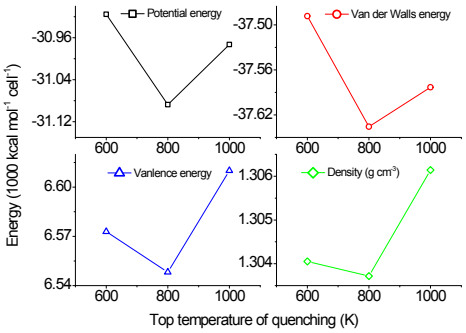


Figure S3 Final energy and density of the equilibrium procedures under 600, 800 and 1000 K as top temperatures of the quenching.

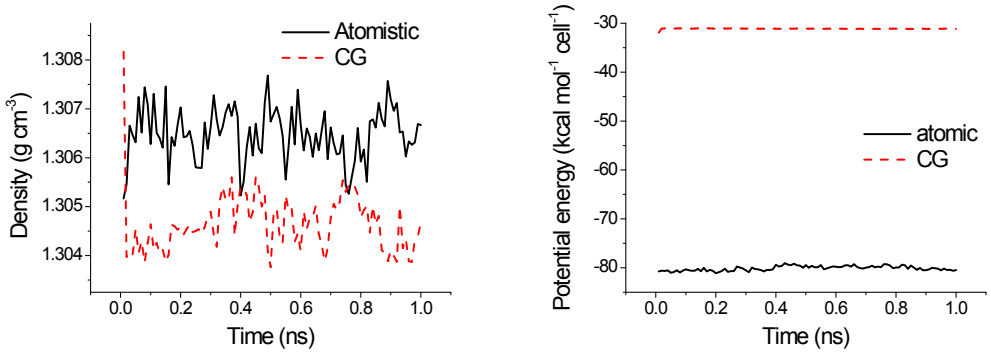
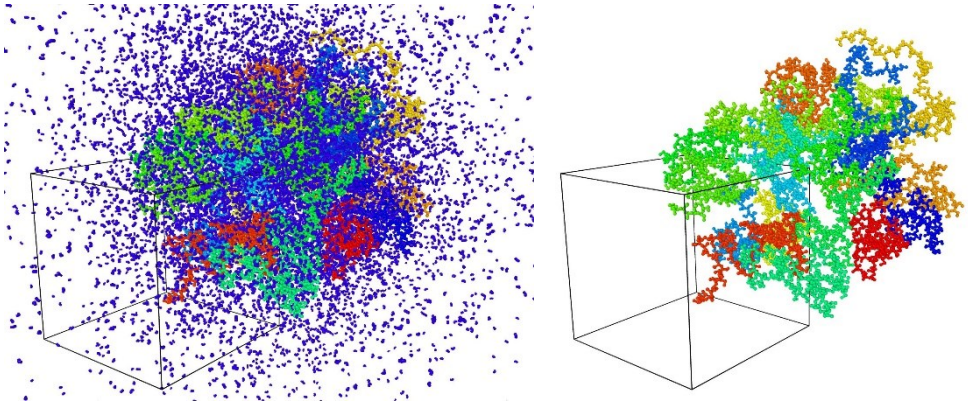
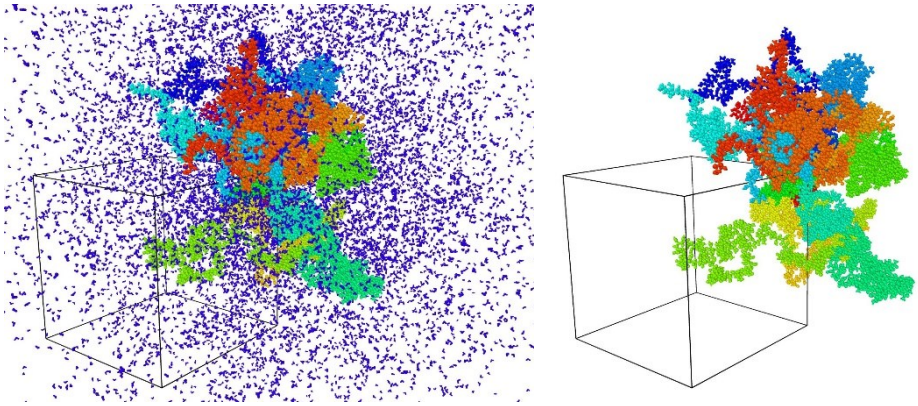


Figure S4 Density and potential energy evolution for the compressed atomistic and CG-PAM melt models.



40% CG-PAM gel 40% CG-PAM gel with water hidden



40% atomistic-PAM gel 40% atomistic-PAM gel with water hidden

Figure S5 View of the 40% atomistic and CG-PAM gel models. The models are under equilibrium.

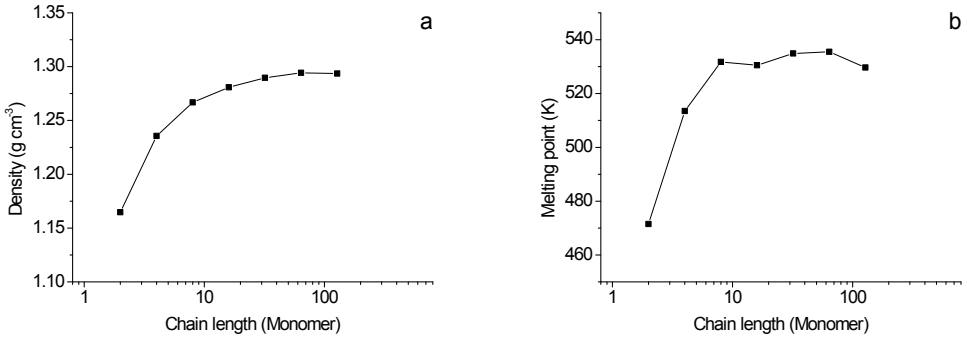


Figure S6 Chain length dependence of density and melting point of CG-PAM melt.