Optimizing the charge transport in redox-active gels: a computational study

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Supplementary Materials

Charge hop events were identified by the change of the host bead occupied by the charge during the simulation. The plots present the total number of hops detected in trajectories collected for 100'000 timesteps long simulations with time resolution (dumping period) 1000 timesteps. Due to technical limitations, consecutive charge hops separated by less than 1000 timesteps may not be resolved. On the other hand, these data do include 'back and forth' charge hops between the closely located 'redox-active' beads, which have little effect on the mean squared displacement curves. Moreover, in contrast to the diffusion process in crystal lattice, the accepting sites ('redox-active' beads) are not evenly distributed and are not fixed in space. Therefore, charge hops frequency provides only crude characterization of charge diffusion in redox-active gel.
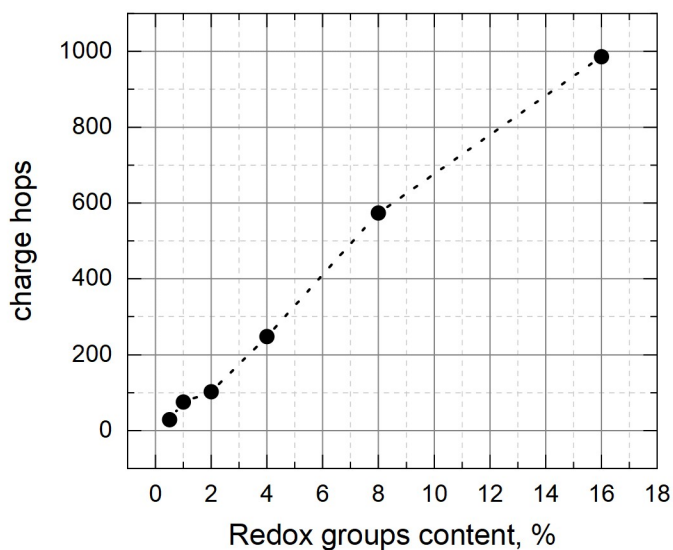

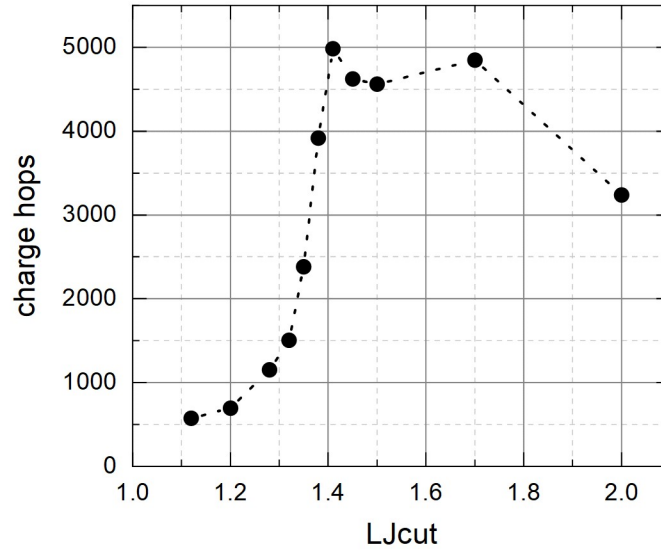Figure S1. The number of detected charge hops for different values of redox groups content.

Figure S2. Number of detected charge hops for different values of Lennard-Jones cut-off distance.

In order to check the presence of enhanced polymer chain fluctuations near the theta-point we have calculated the probability density function (PDF) of local beads concentration across all the beads for various solvent quality conditions (which is controlled by Lennard-Jones potential cutoff) – see figure S3. The local beads concentration was calculated as an average concentration of neighbor beads inside a sphere of radius R = 3 centered at the selected bead. Near the theta point (LJcut = 1.32) the PDF reaches the maximum width. This can be interred as coexisting of regions with different density values.
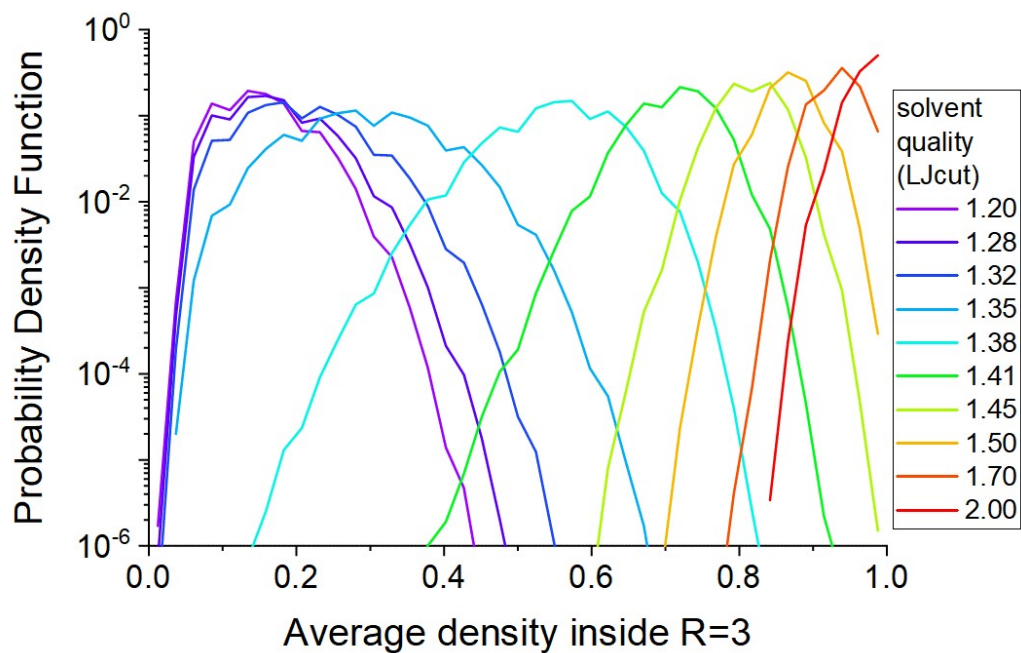

Figure S3. Probability distribution functions of the local density for various solvent quality conditions.