Evidence for Protein Misfolding in the Presence of Nanoplastics

Supporting Information

Oldamur Hollóczki[a,*]

[a]Mulliken Center for Theoretical Chemistry, University of Bonn, Beringstr. 4+6, D-53115 Bonn, Germany

*holloczki@gmail.com

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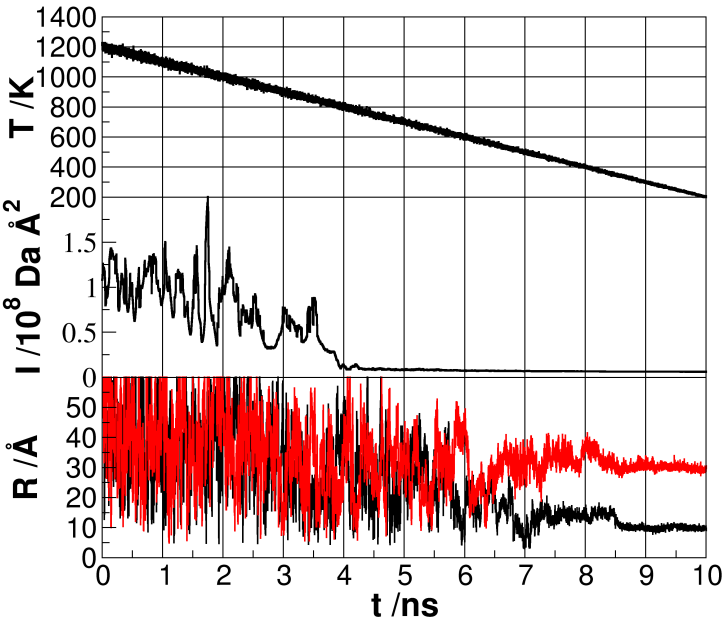

Figure 1: Development of the temperature (T, above), and the structure of 8 $C_{156}H_{288}N_{26}O_{27}$ chains in a simulation box over the 10 ns molecular dynamics simulation. The moment of inertia-like quantity I is defined according to Eq. 2 in the main article, and characterizes the spatial extent of the system (I, middle). The development of intramolecular distances between the terminal carbon atoms of two selected chains shows the mobility of the molecules in the system, and the changes in their capacity to rearrange as the temperature is decreasing (R, below).

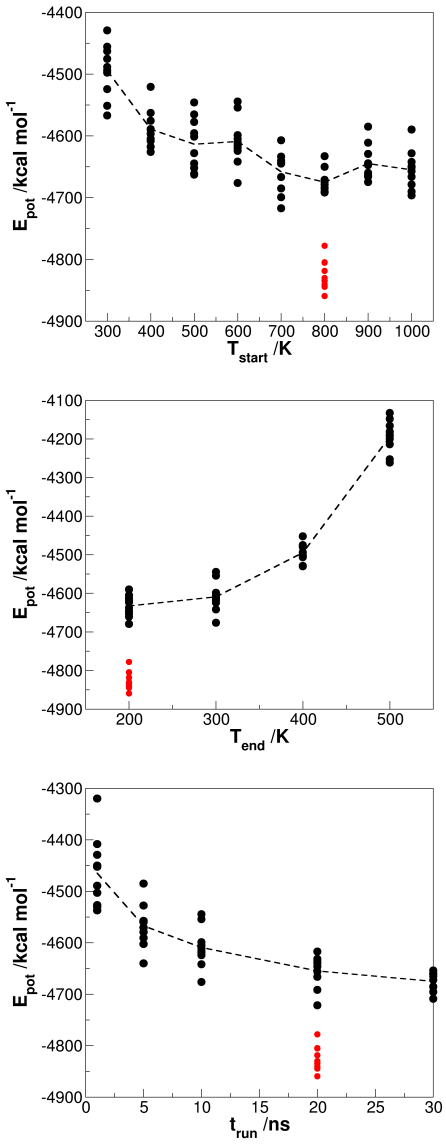

Figure 2: OPLS-AA potential energies of the nylon 6,6 nanoparticles obtained at different T_{start} (top), T_{end} (middle) and t_{run} (bottom) for ten separate starting structures. In the simulations only one parameter was altered from the default $T_{start} = 600\,\mathrm{K}$, $T_{end} = 300\,\mathrm{K}$ and $t_{run} = 10\,\mathrm{ns}$ settings. The dashed lines connect the average values obtained for each setting. The red points show the potential energies for the optimized $T_{start} = 800\,\mathrm{K}$, $T_{end} = 200\,\mathrm{K}$ and $t_{run} = 20\,\mathrm{ns}$ setup.