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

Electronic Supplementary Information

Multiscale Simulations of Ligand Adsorption and Exchange on Gold Nanoparticles

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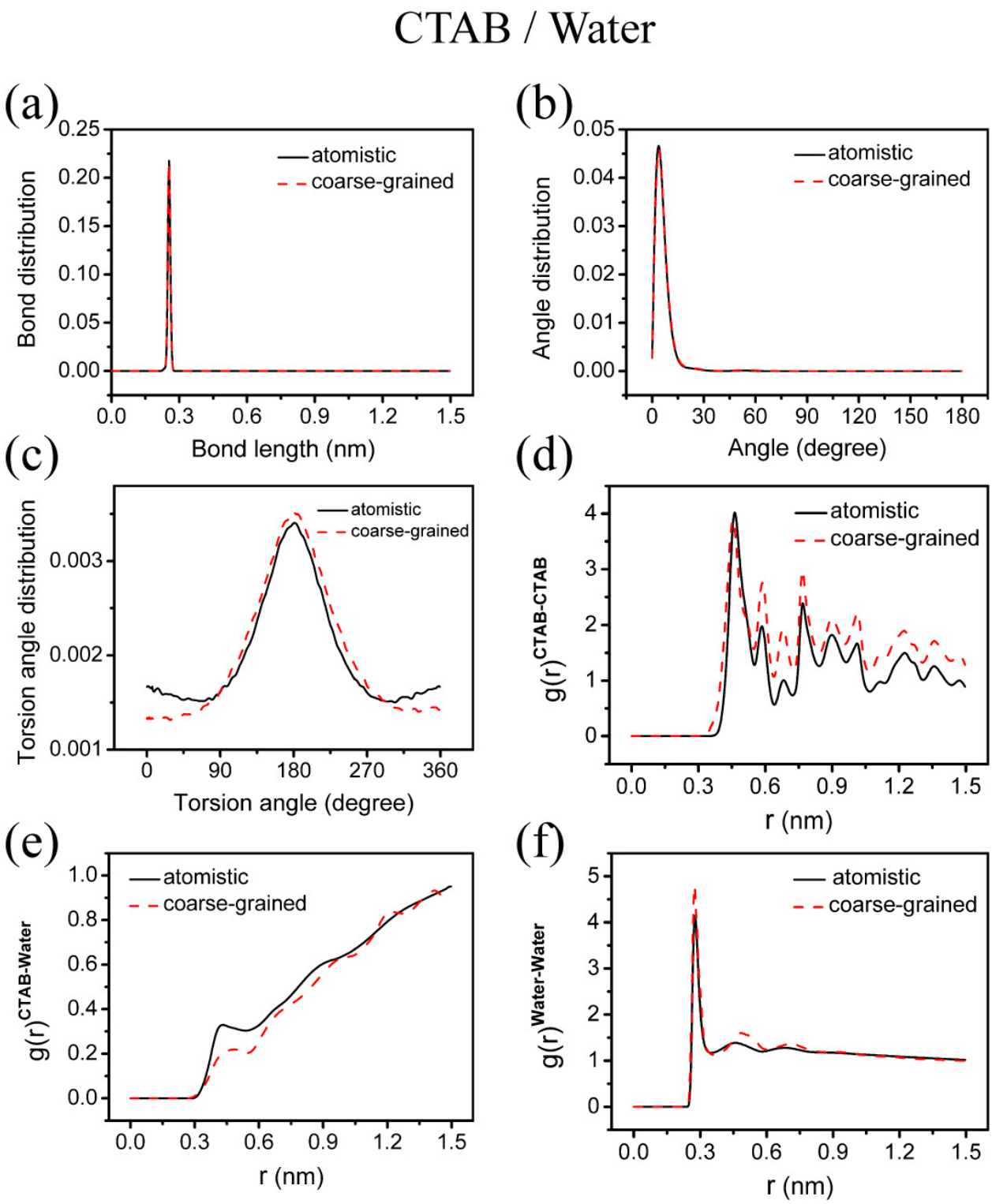

Figure S1: Calculated bonded distribution and nonbonded radial distribution functions (RDF) between centers of mass of monomers from atomistic and coarse-grained simulations of CTAB in water at 298 K. Bonded distribution: (a) bond lengths, (b) angle, and (c) torsion angles. Nonbonded RDF: (d) CTAB-CTAB, (e) CTAB-Water, and (f) Water-Water. The concentration of CTAB is 40 mon %. All bonded and nonbonded interactions are in acceptable agreement with the target distribution functions.

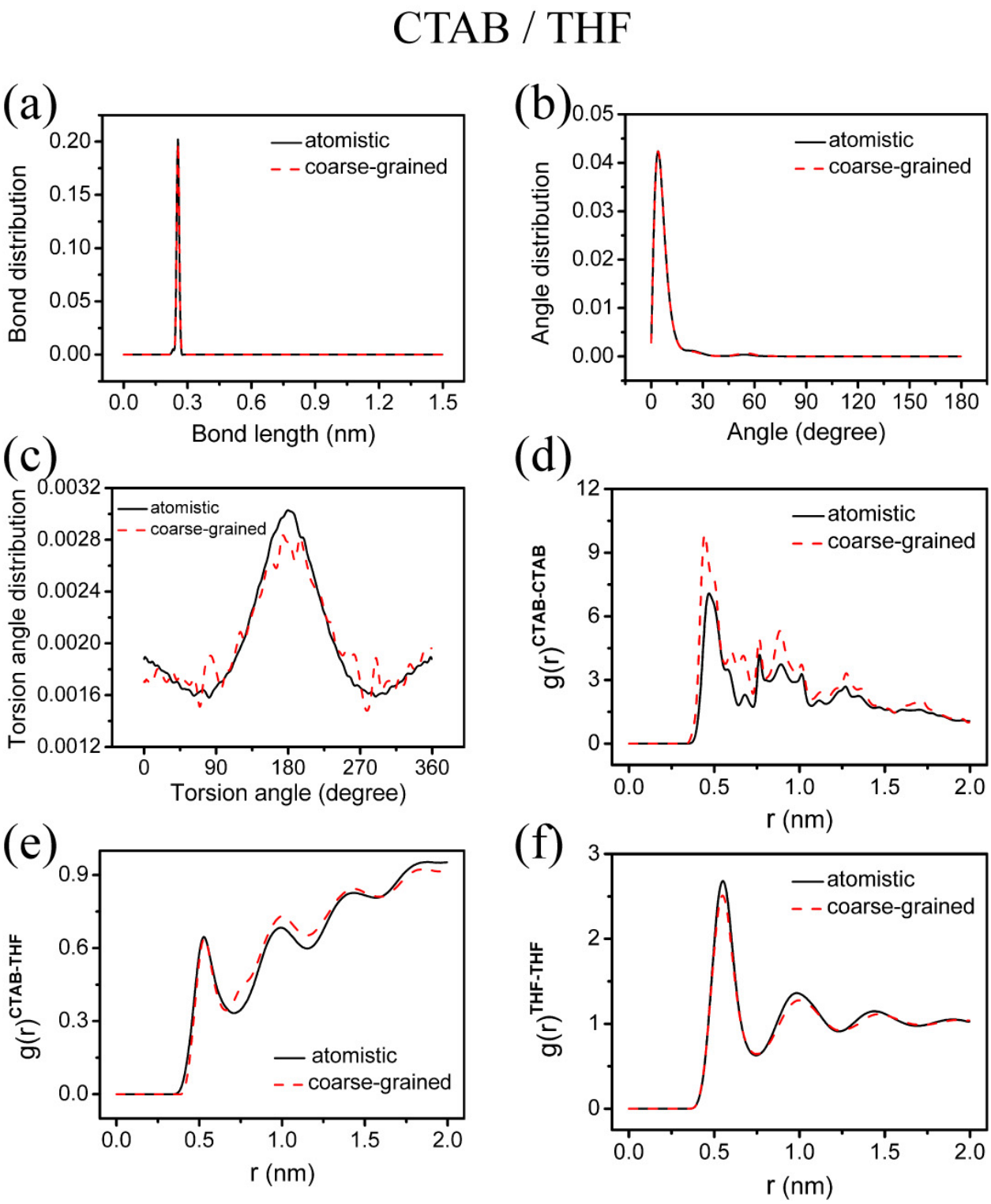

Figure S2: Calculated bonded distribution and nonbonded radial distribution functions (RDF) between centers of mass of monomers from atomistic and coarse-grained simulations of CTAB in THF at 298 K. Bonded distribution: (a) bond lengths, (b) angle, and (c) torsion angles. Nonbonded RDF: (d) CTAB-CTAB, (e) CTAB-THF, and (f) THF-THF. The concentration of CTAB is 40 mon %. All bonded and nonbonded interactions are in acceptable agreement with the target distribution functions.

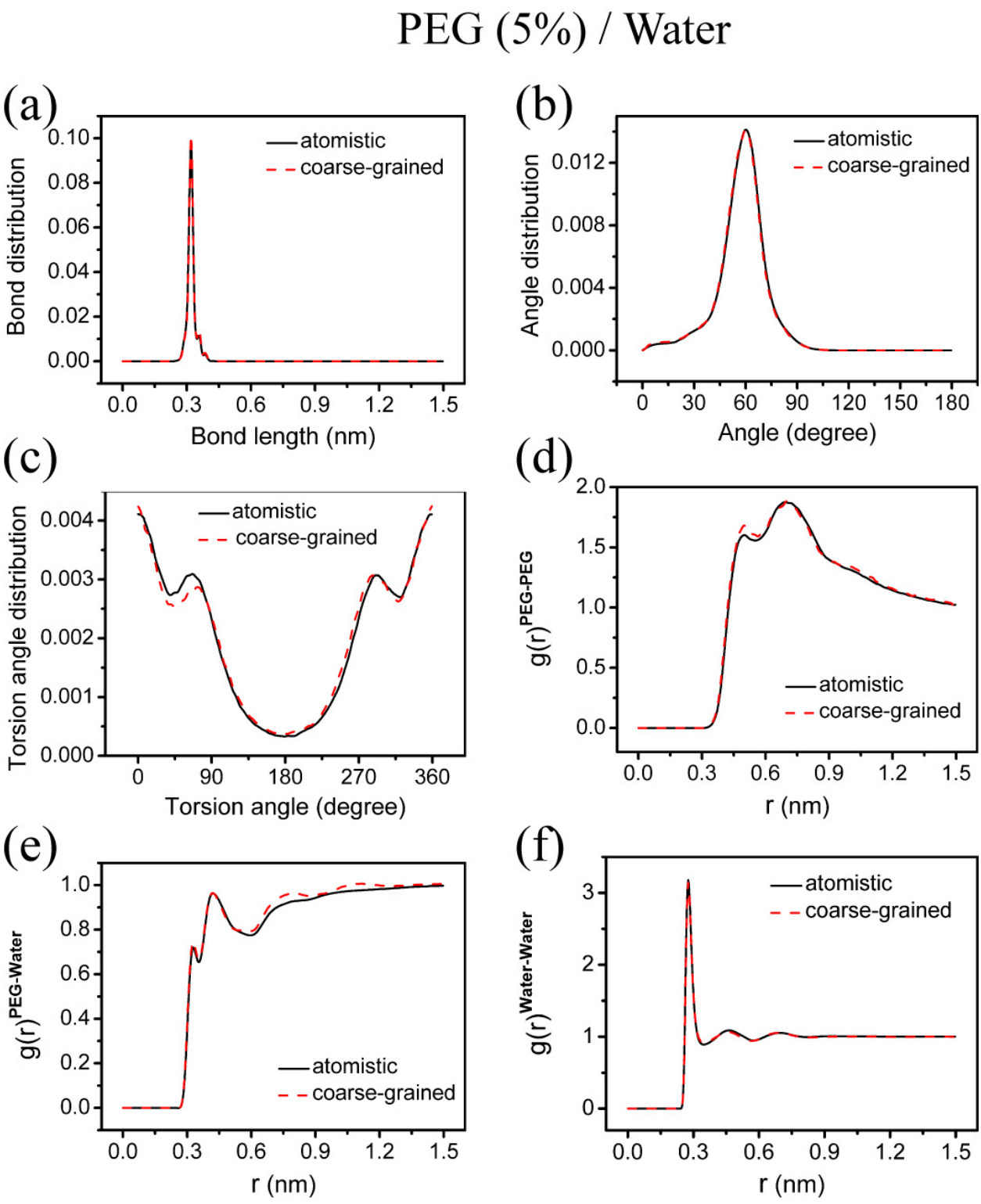

Figure S3: Calculated bonded distribution and nonbonded radial distribution functions (RDF) between centers of mass of monomers from atomistic and coarse-grained simulations of PEG11 in water at 298 K. Bonded distribution: (a) bond lengths, (b) angle, and (c) torsion angles. Nonbonded RDF: (d) PEG-PEG, (e) PEG-Water, and (f) Water-Water. The concentration of PEG is 5 mon %. All bonded and nonbonded interactions are in acceptable agreement with the target distribution functions.

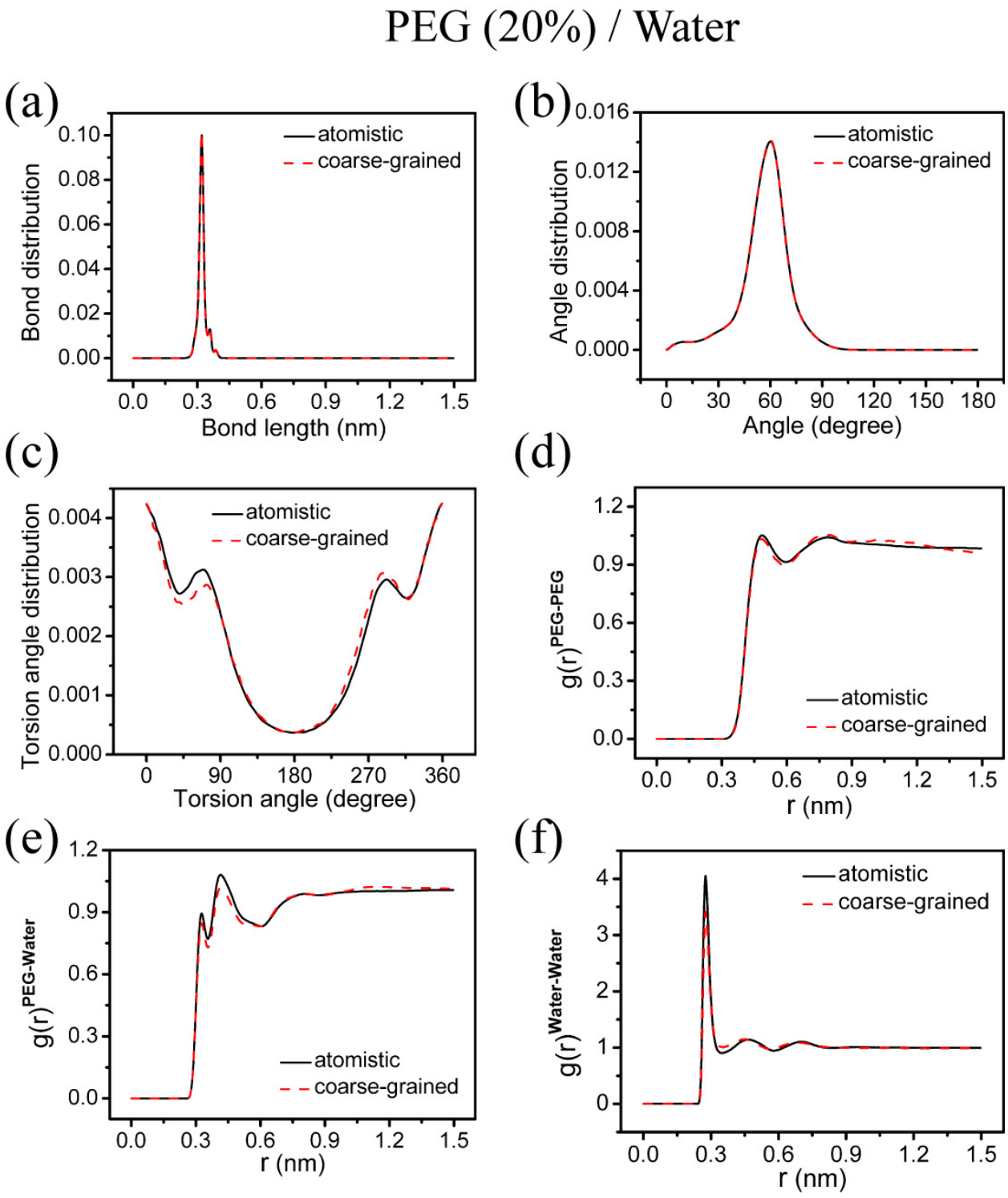

Figure S4: Calculated bonded distribution and nonbonded radial distribution functions (RDF) between centers of mass of monomers from atomistic and coarse-grained simulations of PEG11 in water at 298 K. Bonded distribution: (a) bond lengths, (b) angle, and (c) torsion angles. Nonbonded RDF: (d) PEG-PEG, (e) PEG-Water, and (f) Water-Water. The concentration of PEG is 20 mon %. All bonded and nonbonded interactions are in acceptable agreement with the target distribution functions.

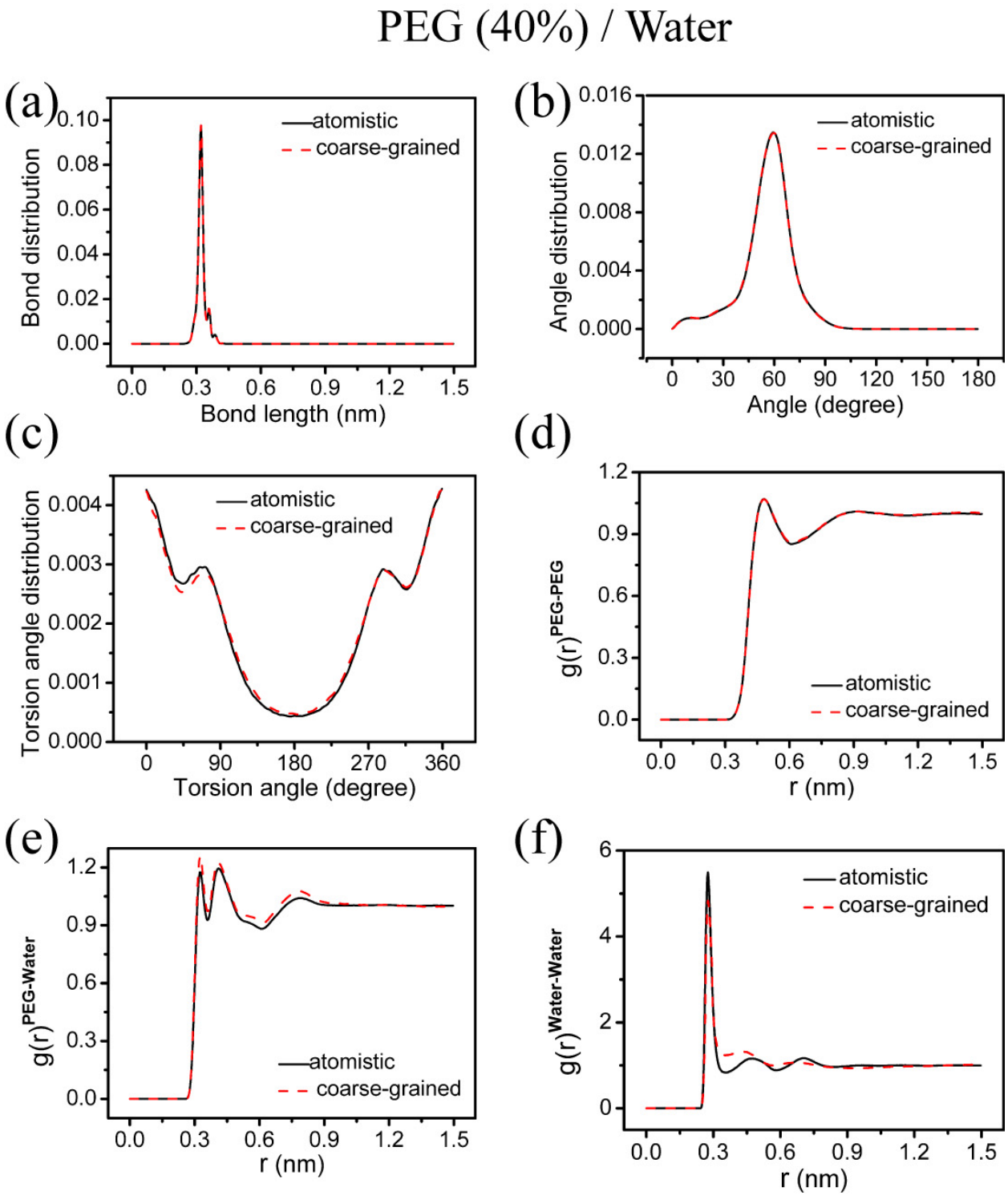

Figure S5: Calculated bonded distribution and nonbonded radial distribution functions (RDF) between centers of mass of monomers from atomistic and coarse-grained simulations of PEG11 in water at 298 K. Bonded distribution: (a) bond lengths, (b) angle, and (c) torsion angles. Nonbonded RDF: (d) PEG-PEG, (e) PEG-Water, and (f) Water-Water. The concentration of PEG is 40 mon %. All bonded and nonbonded interactions are in acceptable agreement with the target distribution functions.

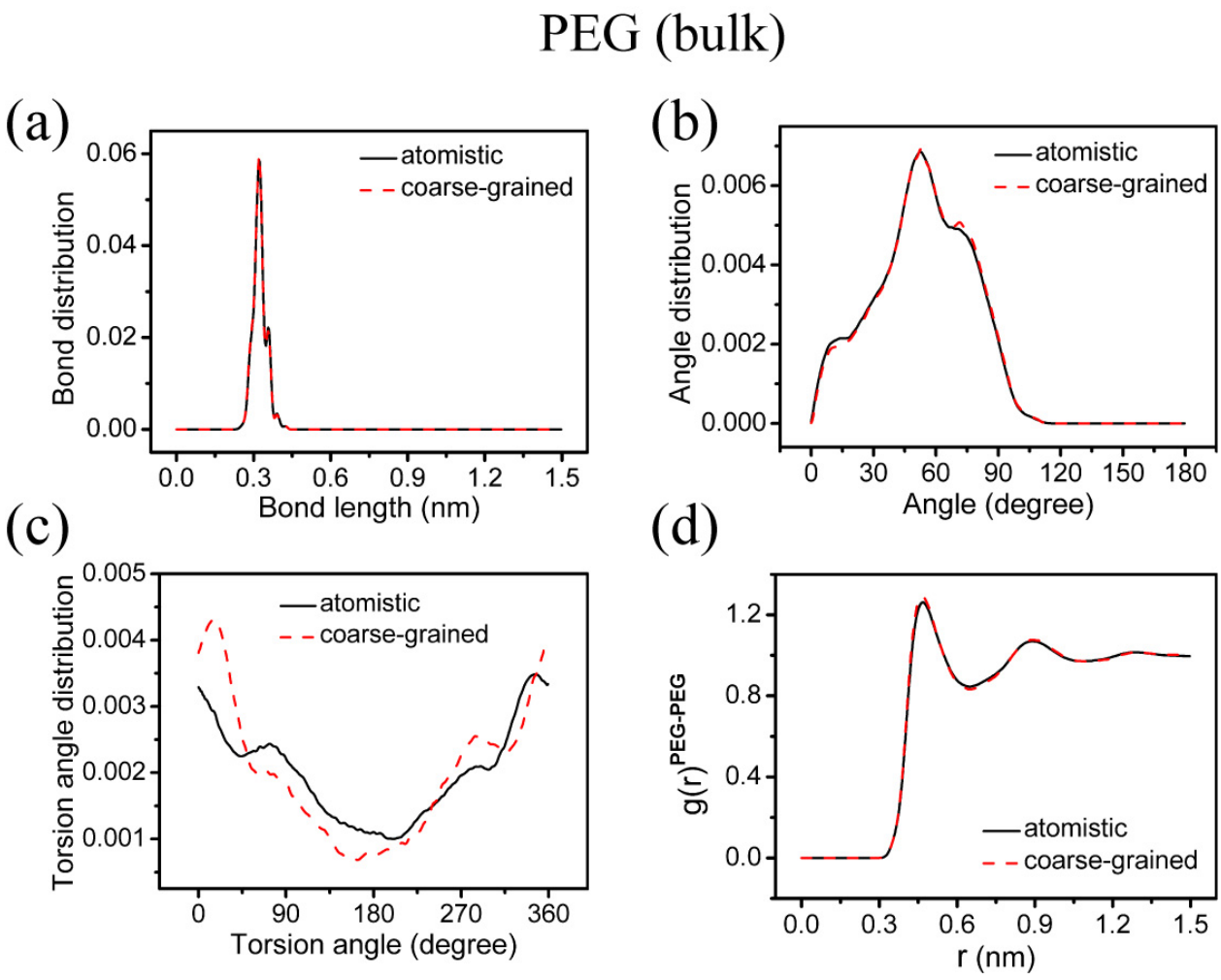

Figure S6: Calculated bonded distribution and nonbonded radial distribution functions (RDF) between centers of mass of monomers from atomistic and coarse-grained simulations of PEG11 bulk at 298 K. (a) Bond length distribution, (b) angle distribution, (c) torsion angle distribution, and (d) nonbonded RDF between PEG-PEG. All bonded and nonbonded interactions are in acceptable agreement with the target distribution functions.

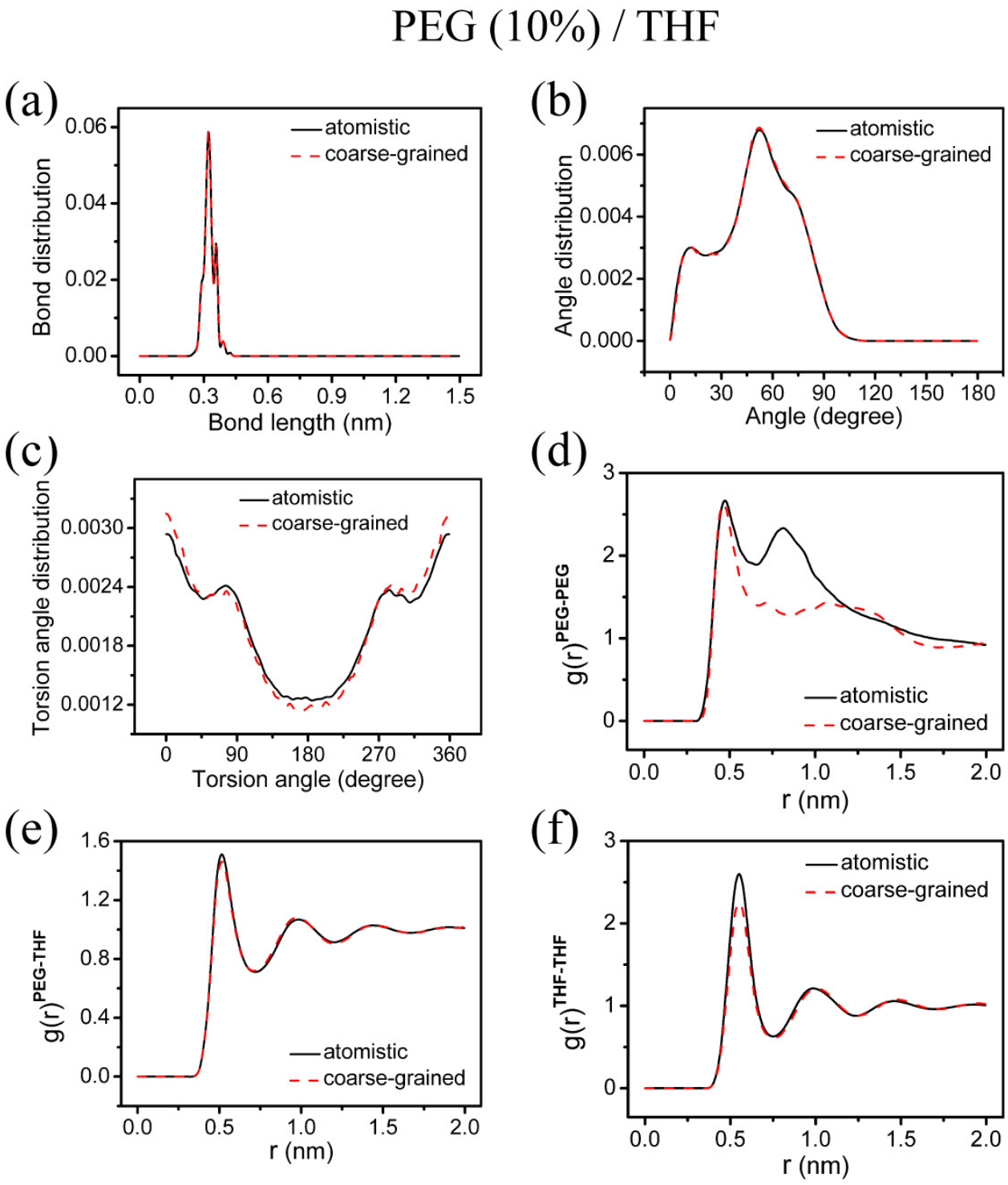

Figure S7: Calculated bonded distribution and nonbonded radial distribution functions (RDF) between centers of mass of monomers from atomistic and coarse-grained simulations of PEG11 in THF at 298 K. Bonded distribution: (a) bond lengths, (b) angle, and (c) torsion angles. Nonbonded RDF: (d) PEG-PEG, (e) PEG-THF, and (f) THF-THF. The concentration of PEG is 10 mon %. All bonded and nonbonded interactions are in acceptable agreement with the target distribution functions.

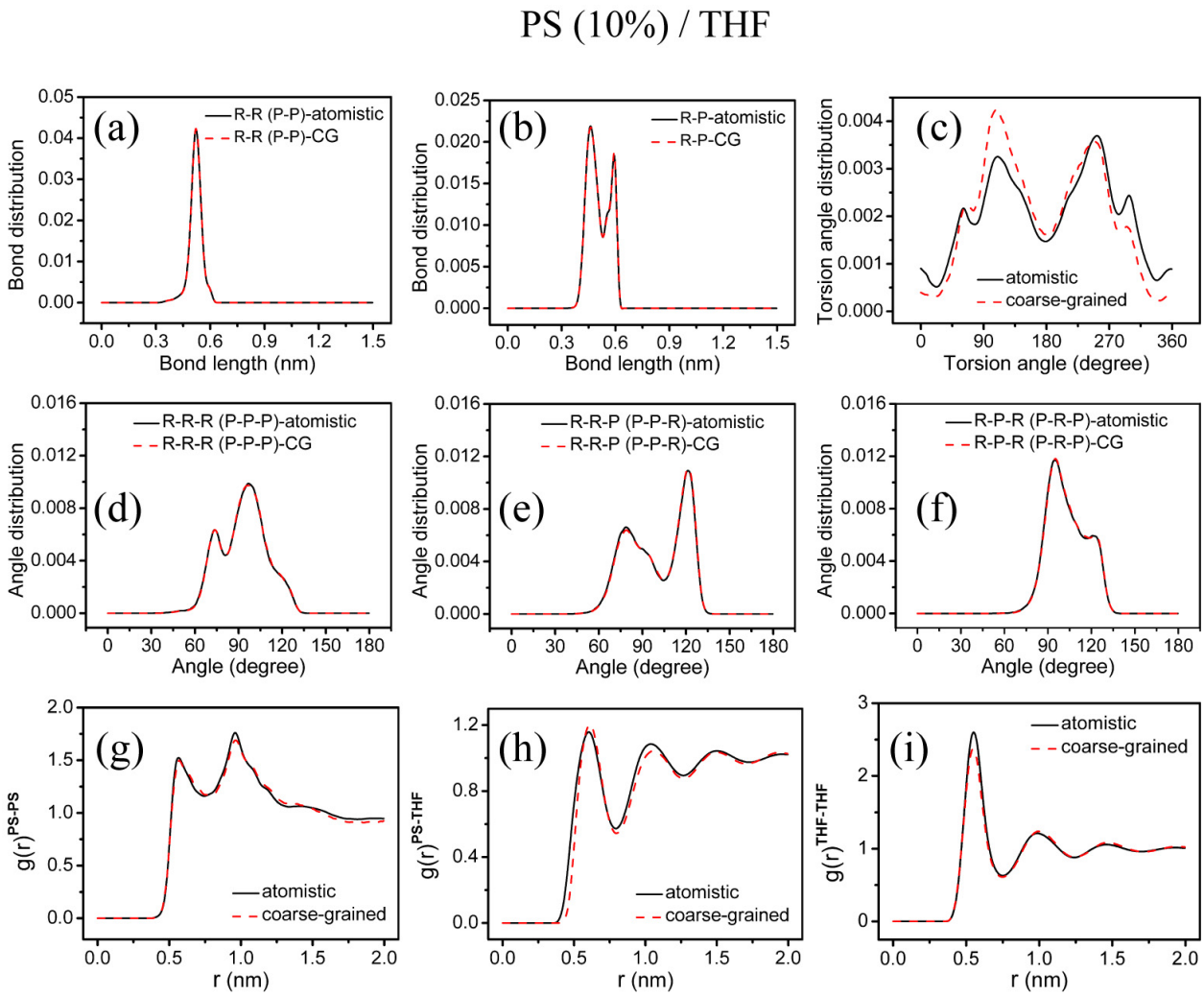

Figure S8: Calculated bonded distribution and nonbonded radial distribution functions (RDF) between centers of mass of monomers from atomistic and coarse-grained simulations of PS10 in THF at 298 K. (a) Bond length distribution for $R-R$, (b) bond length distribution for $R-P$, (c) torsion angle distribution, (d) angle distribution for $R-R-R$, (e) angle distribution for $R-R-P$, (f) angle distribution for $R-P-R$, and nonbonded RDF between (g) PS-PS, (h) PS-THF, and (i) THF-THF. The concentration of PS is 10 mon %. All bonded and nonbonded interactions are in acceptable agreement with the target distribution functions.

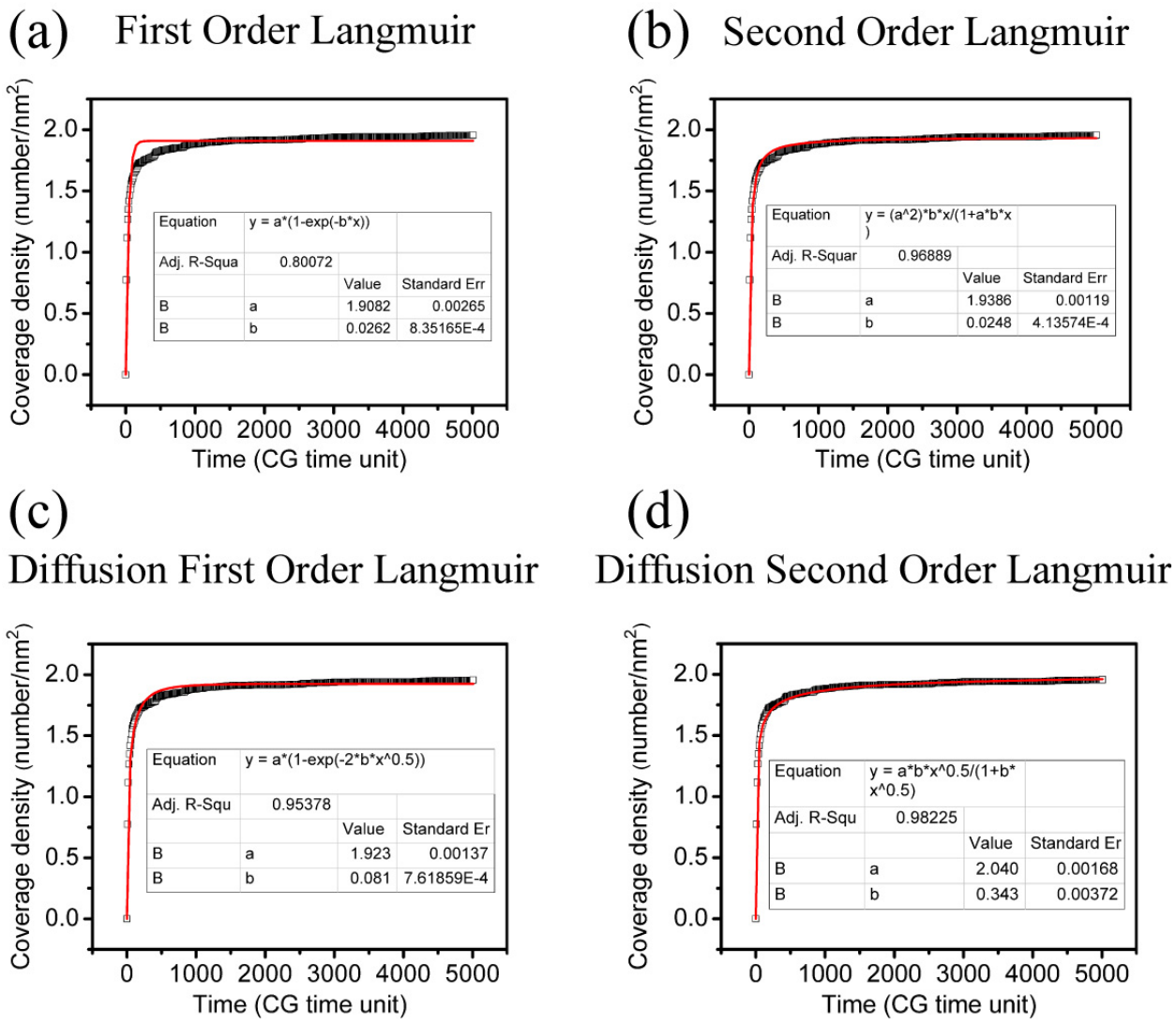

Figure S9: Adsorption kinetics of CTAB on gold surfaces in water. The curves represent model fit for (a) first order Langmuir (1*L*), (b) second order Langmuir (2*L*), (c) diffusion-limited first order Langmuir (1*LD*), and (d) diffusion-limited second order Langmuir (2*LD*). Fitting to traditional first order reaction yields unsatisfactory results, while the diffusion-limited second order Langmuir (2*LD*) kinetic offers the best description of the data.

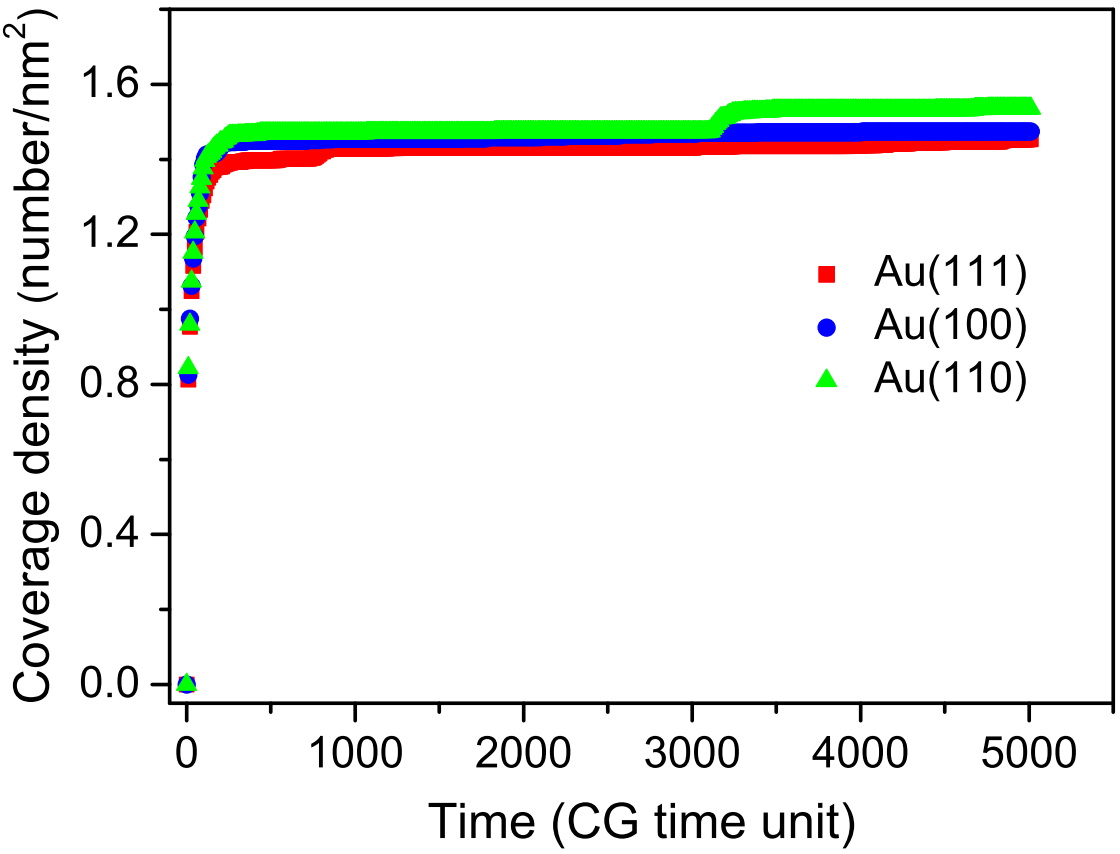

Figure S10: The coverage density for CTAB molecules in THF on Au(111), Au(100) and Au(110) surfaces.