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

Supporting Information: Simple corrections for the static dielectric constant of liquid mixtures from model force fields

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1 Static dielectric constant

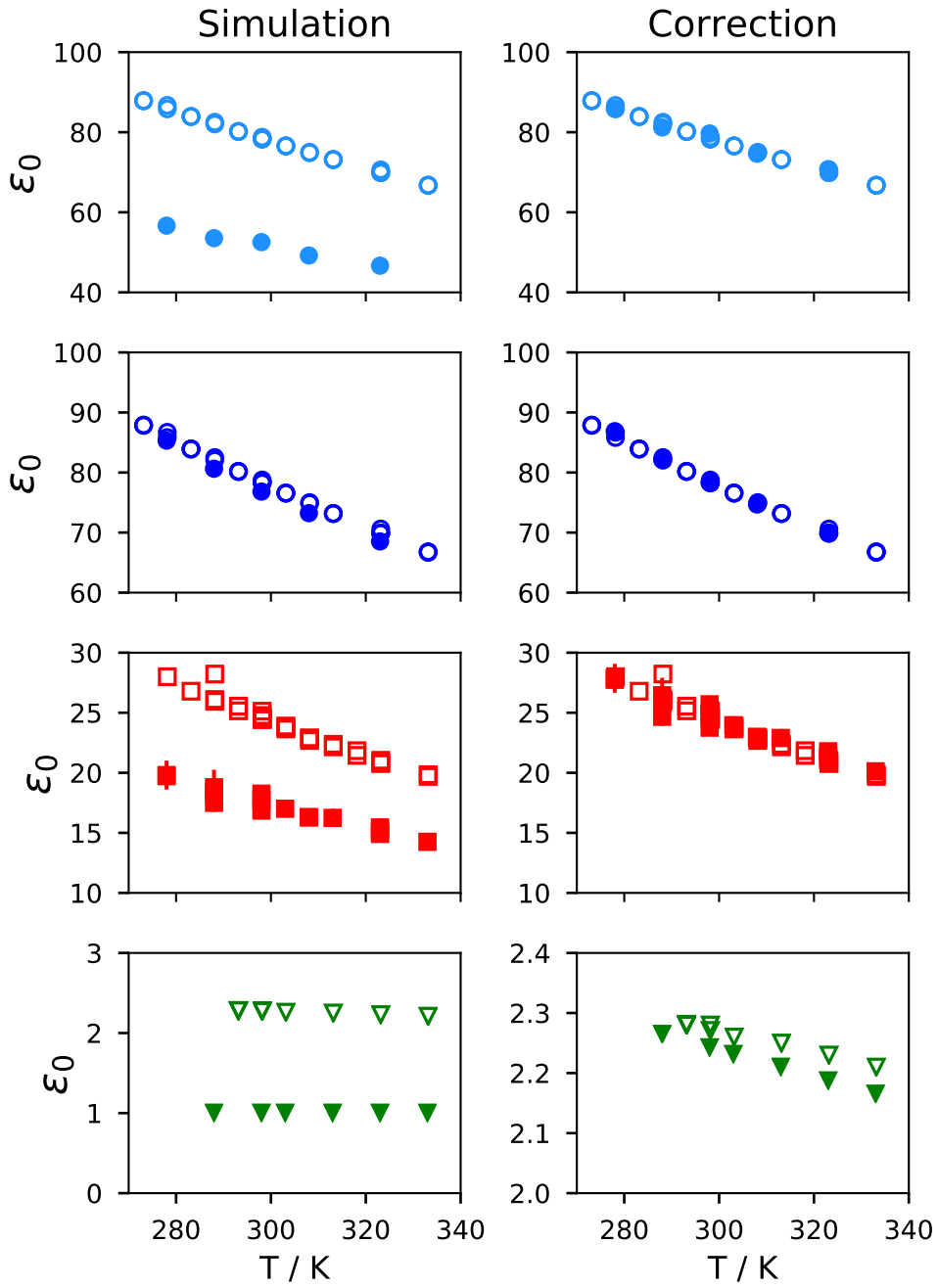

Figure S1: Influence of temperature on the static dielectric constant ε_0 of water (TIP4P, light blue), water (SPC-Fw, dark blue), ethanol (TraPPE-UA, red) and benzene (TraPPE-EH, green) at 1 bar. Filled symbols represent results obtained in our original simulations (left) and after applying the proposed correction scheme (right). Open symbols correspond to experimental measurements from different sources for water,[S1–S6] ethanol,[S1,S5–S10] and benzene.[S6,S11–S14]

2 Dipole moment distributions

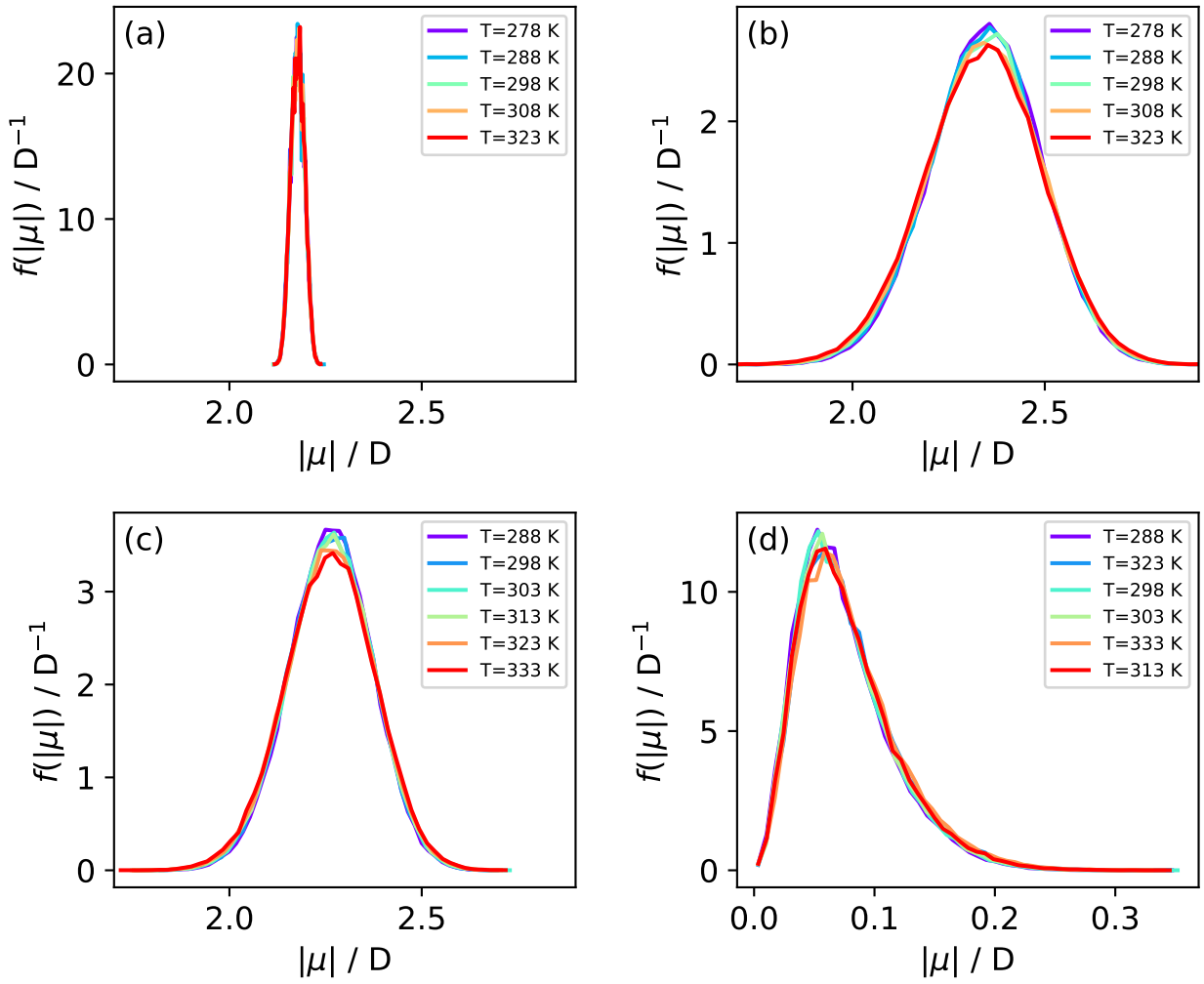

Figure S2: Influence of temperature on the dipole moment distribution of (a) water TIP4P, (b) water SPC-Fw, (c) ethanol TraPPE-UA and (d) benzene TraPPE-EH at 1 bar.

3 Temperature dependence of simulated static dielectric constant and infinite frequency dielectric constant

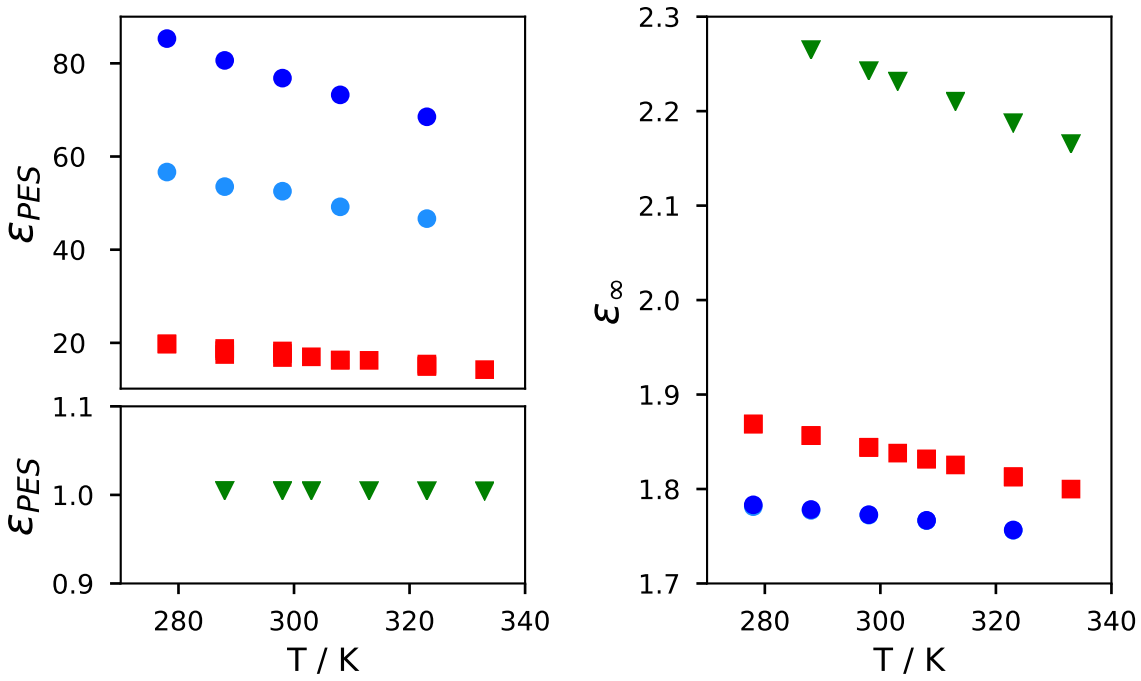

Figure S3: Influence of temperature on the simulated static dielectric constant ε_{PES} (left) and infinite frequency dielectric constant ε_{∞} (right) of water (TIP4P, light blue), water (SPC-Fw, dark blue), ethanol (TraPPE-UA, red) and benzene (TraPPE-EH, green) at 1 bar. The data points corresponding to water TIP4P and SPC-Fw for ε_{∞} overlap and only the latter are visible on the figure.

4 Density

4.1 Single components

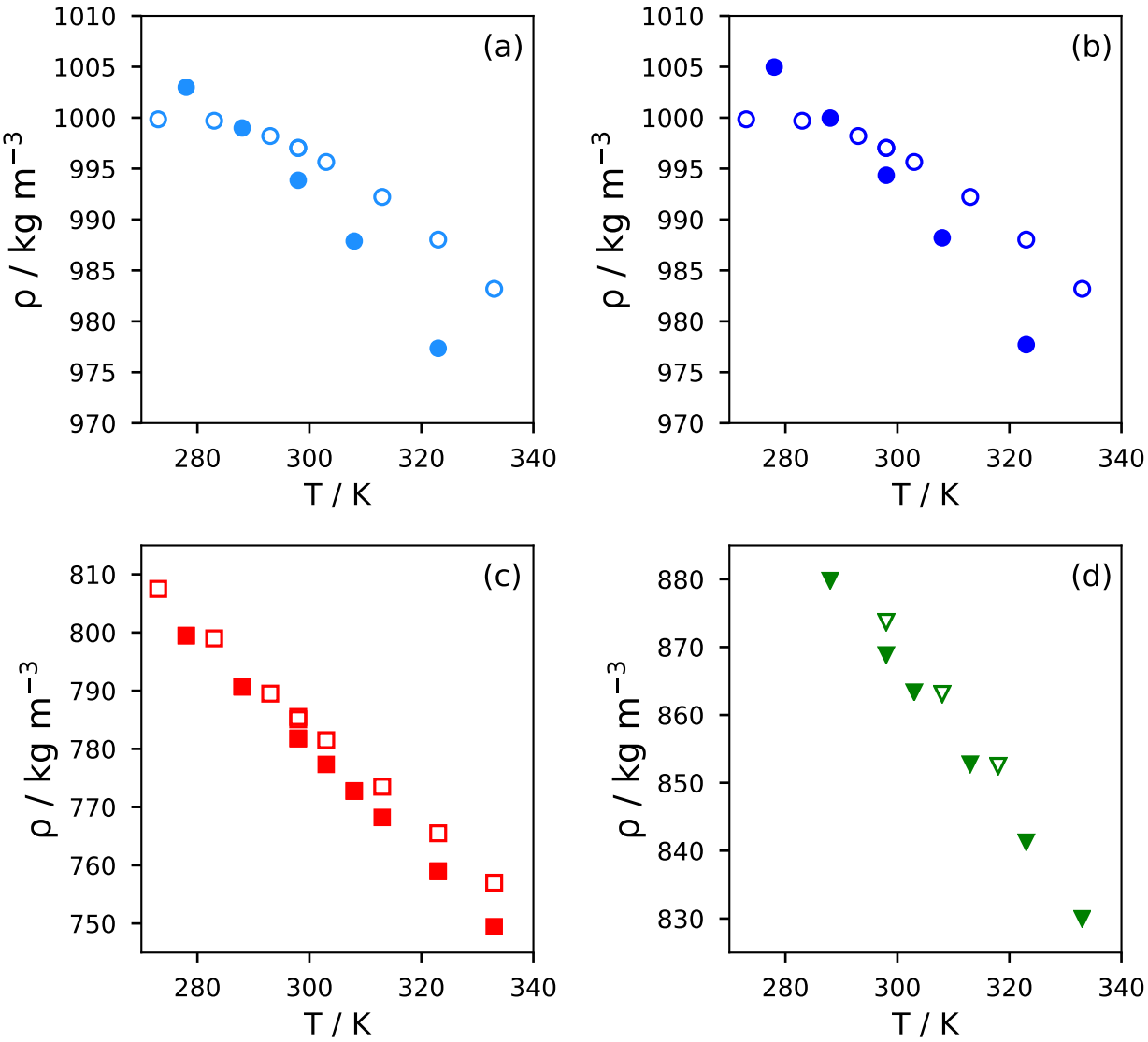

Figure S4: Influence of temperature on the density of (a) water TIP4P, (b) water SPC-Fw, (c) ethanol TraPPE-UA and (d) benzene TraPPE-EH at 1 bar. Filled symbols represent results obtained in our simulations. Open symbols correspond to experimental measurements for water,[S9,S15] ethanol,[S9,S15] and benzene.[S16]

4.2 Mixtures

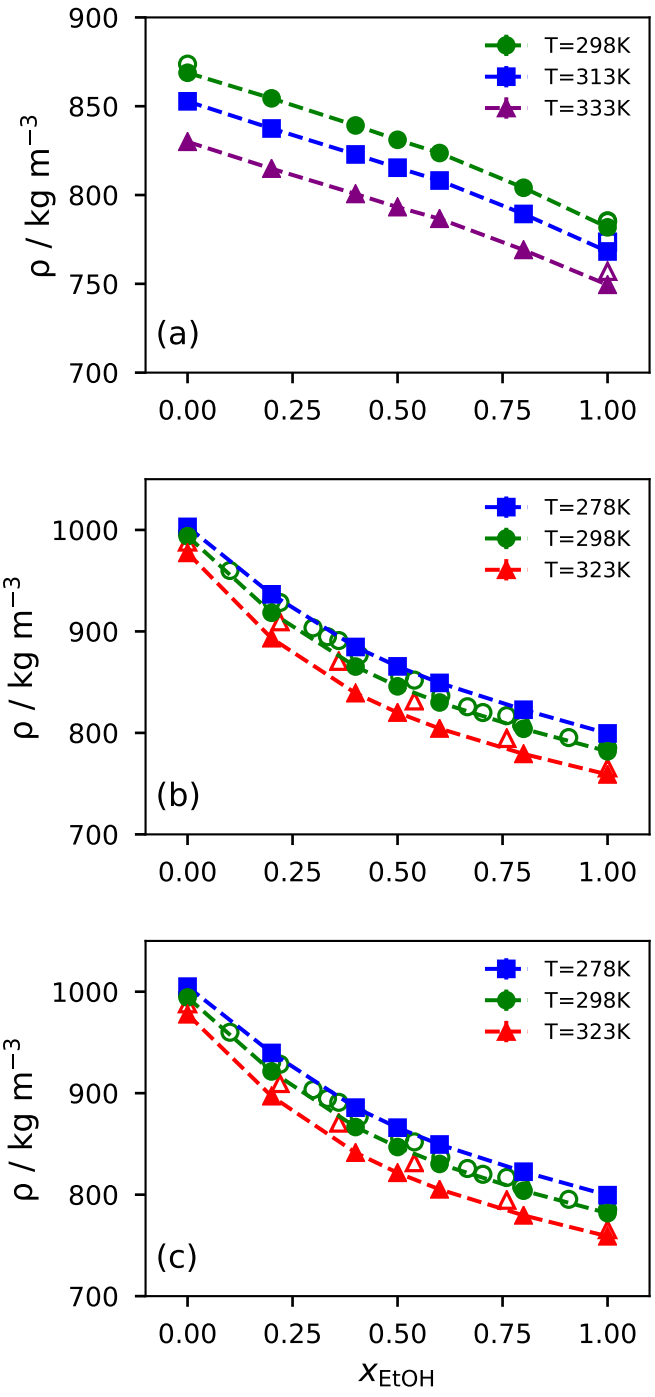

Figure S5: Influence of temperature on the density of (a) ethanol-benzene, (b) ethanol-water TIP4P, and (c) ethanol-water SPC-Fw mixtures at 1 bar. Filled symbols represent results obtained in our simulations. Open symbols correspond to experimental measurements for ethanol-benzene[S9,S15,S16] and ethanol-water[S9,S15] mixtures.

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