Supplementary Material for "Symmetry-preserving mean field theory for electrostatics at interfaces"

Zhonghan Hu[1,2,*]

[1]*State Key Laboratory of Supramolecular Structure and Materials, Jilin University, Changchun, 130012, P. R. China*

[2]*Institute of Theoretical Chemistry, Jilin University, Changchun, 130012, P. R. China*

Abstract

*Electronic address: zhonghanhu@jlu.edu.cn

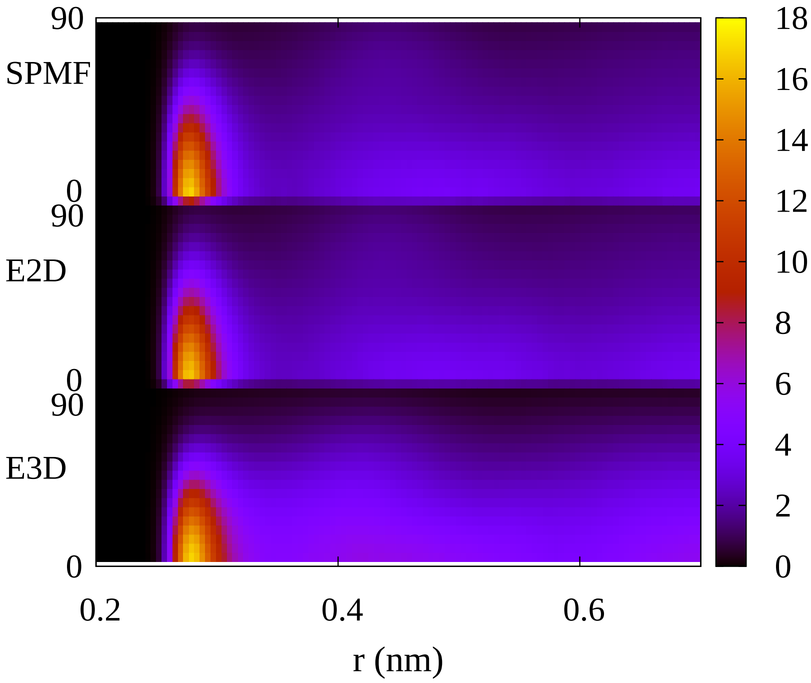

FIG. S1: The radial angle distributions, $g(r, \theta)$ at $E_0 = 20\mathrm{Volts/nm}$ using SPMF (top),the Ewald2D method (middle) and the Ewald3D method (bottom). No significant differences are found among three contour plots because the correlations are mainly determined by the short-ranged interactions and less affected by the long-ranged component of the electrostatic interactions.

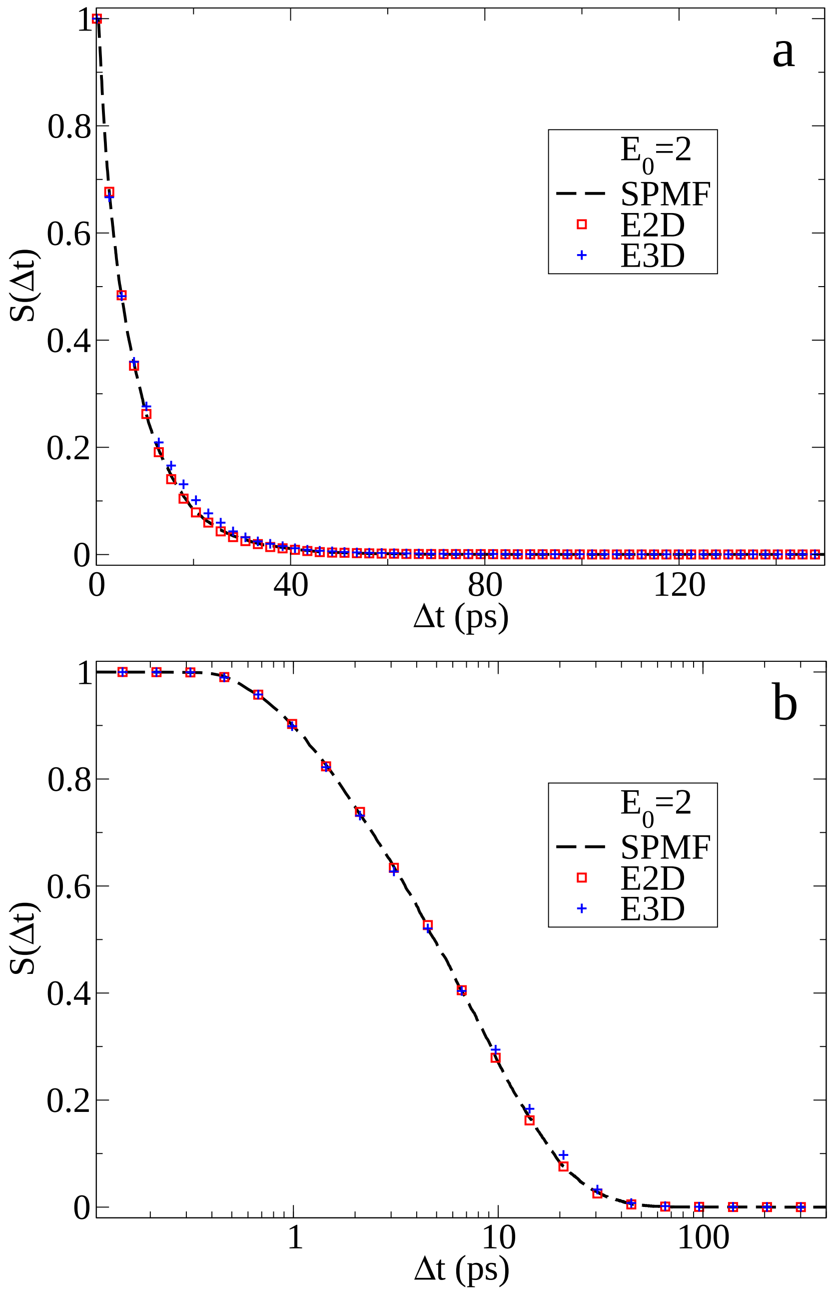

FIG. S2: The survival probabilities $S(\Delta t)$ at $E_0 = 2\mathrm{Volts/nm}$ using SPMF (dash line),the Ewald2D method (open square) and the Ewald3D method (plus) plotted in the linear (a) and the logarithmic (b) time scale. This survival probability, $S(\Delta t) = P(z(\Delta t) < z_b | z(0) \geqslant z_0)$ is the conditional probability of finding the oxygen atom having not passed over the barrier point $z_b = 1.70\mathrm{nm}$ at time Δt given that the oxygen atom is initially located inside the interfacial region $z(0) \geqslant z_0 = 1.85\mathrm{nm}$. The barrier position $z_b = 1.70\mathrm{nm}$ and the well position $z_0 = 1.85\mathrm{nm}$ are determined from the local minimum and maximum of the density distribution close to the interface respectively. There might be very slight difference between the result of SPMF/Ewald2D and the result of Ewald3D. However, it is hard to characterize it using a few independent trajectories.

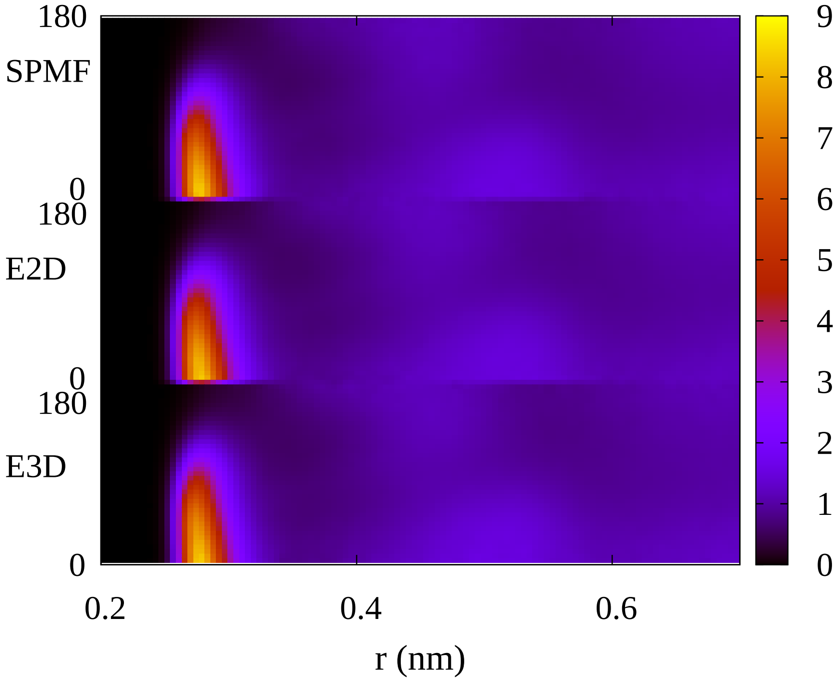

FIG. S3: The radial angle distributions, $g(r, \theta)$ at $E_0 = 2\mathrm{Volts/nm}$ using SPMF (top),the Ewald2D method (middle) and the Ewald3D method (bottom). No notable differences are found among three contour plots.