Solvent Exchange around Aqueous Zn(II) from Ab Initio Molecular Dynamics Simulations

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Supplementary Materials

Figure S1. Cartesian coordinates of the structures from Figure 4.

Figure S1. Cartesian coordinates of the structures from Figure 4.

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Zn(H2O)6
Zn         0.253360         0.315261         0.189336
O          1.503699        -1.174274         1.060860
H          1.875818        -1.598386         0.820582
H          1.824696        -1.256016         1.601447
O          0.738030         1.727175         1.752688
H          0.759336         1.543563         2.496215
H          0.972093         2.309795         1.765409
O          1.921796         1.012758        -0.959669
H          2.635643         0.659472        -0.899453
H          2.076462         1.618935        -1.188246
O         -0.993948         1.747723        -0.800130
H         -1.389373         2.245410        -0.480276
H         -1.014151         1.910229        -1.446292
O         -0.303908        -1.112573        -1.370770
H         -0.920595        -1.153212        -1.685788
H         -0.157771        -1.781664        -1.407024
O         -1.403060        -0.354817         1.395398
H         -2.037265        -0.568862         1.190309
H         -1.494160        -0.283755         2.059145

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Zn(H2O)5
Zn         0.021474         0.036139         0.097448
O         -0.571963         0.975749         1.816309
H         -0.337417         0.544369         2.577913
H         -0.262026         1.888071         1.855534
O          2.004876         0.610860         0.562729
H          2.747457         0.261357         0.094228
H          2.236097         0.934271         1.376621
O          0.288970        -1.960956         0.398454
H          1.110370        -2.192587         0.829633
H          0.229907        -2.539114        -0.364855
O          0.261298         0.711993        -1.783415
H          0.977653         0.944487        -2.206436
H         -0.427984         0.559367        -2.425548
O         -2.062170        -0.282219        -0.391947
H         -2.616915        -0.590783         0.022138
H         -2.430990         0.494893        -0.742004
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