**Supplementary Information**

# A Martini Coarse-Grained Model for Poly(alkylimidazolium) Ionenes and Applications in Aromatic Compound Extraction

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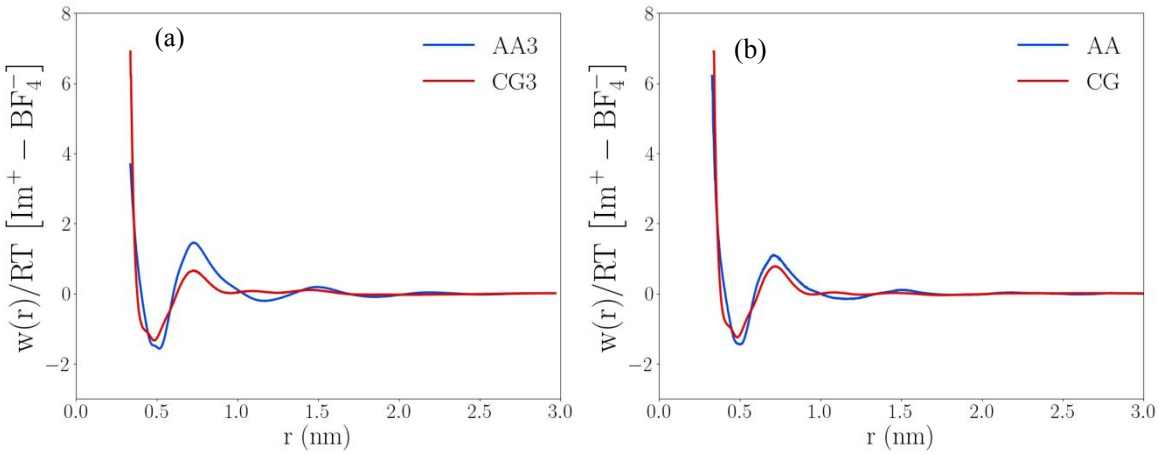


**Figure S1.** PMF of the imidazolium ring ($Im^+$)-[$BF^-_4$] and ($cIm^+$)-[$BF^-_4$] interactions at 298 K and 1 bar, corresponding to systems: (a) AA3 and CG3, and (b) AA4 and CG4. The labels and reference sites are consistent with Figure 3.

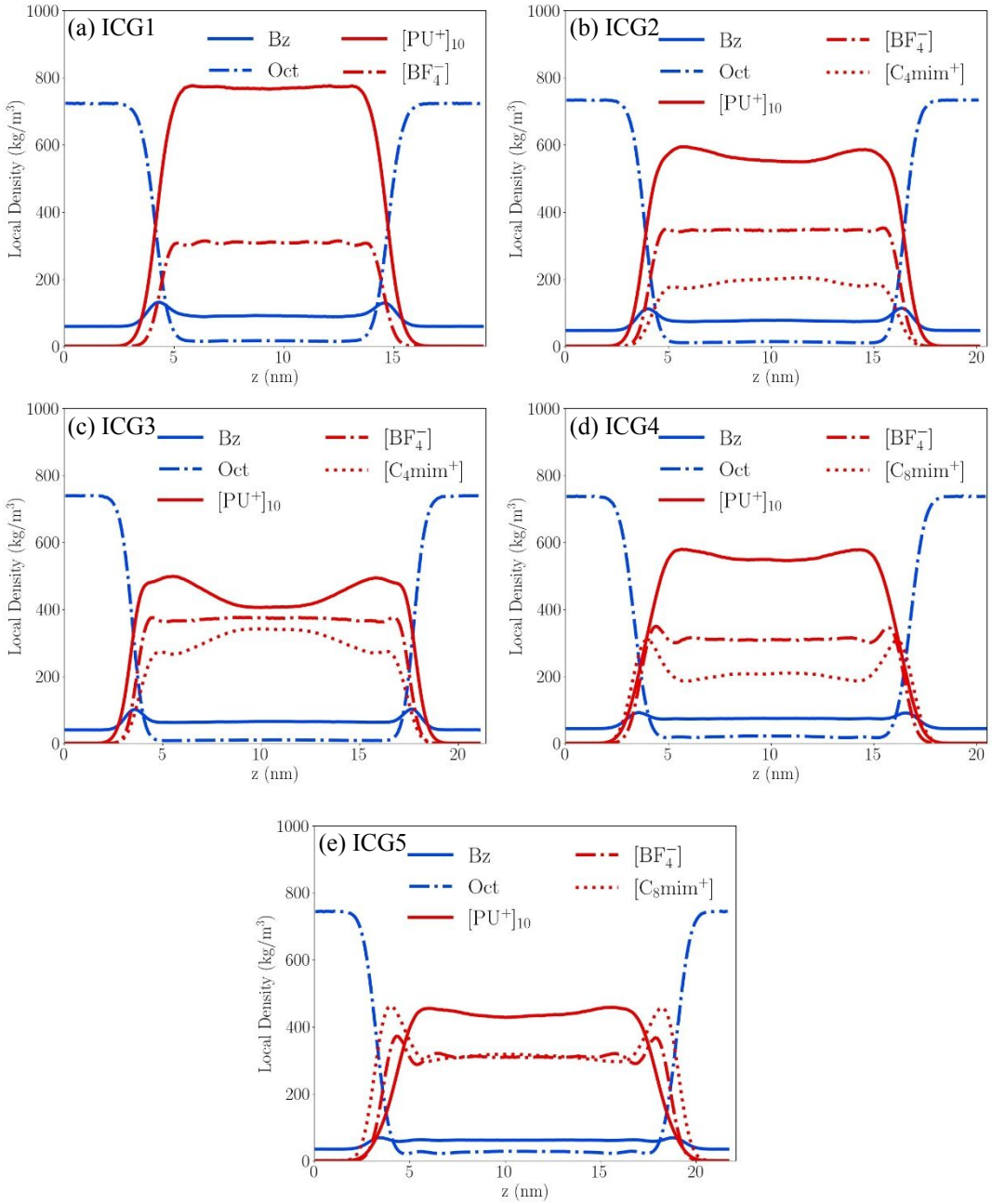


**Figure S2**. Mass local density of the interfacial systems: (a) ICG1, (b) ICG2, (c) ICG3, (d) ICG4, and (e) ICG5 at 298 K and 1 bar.

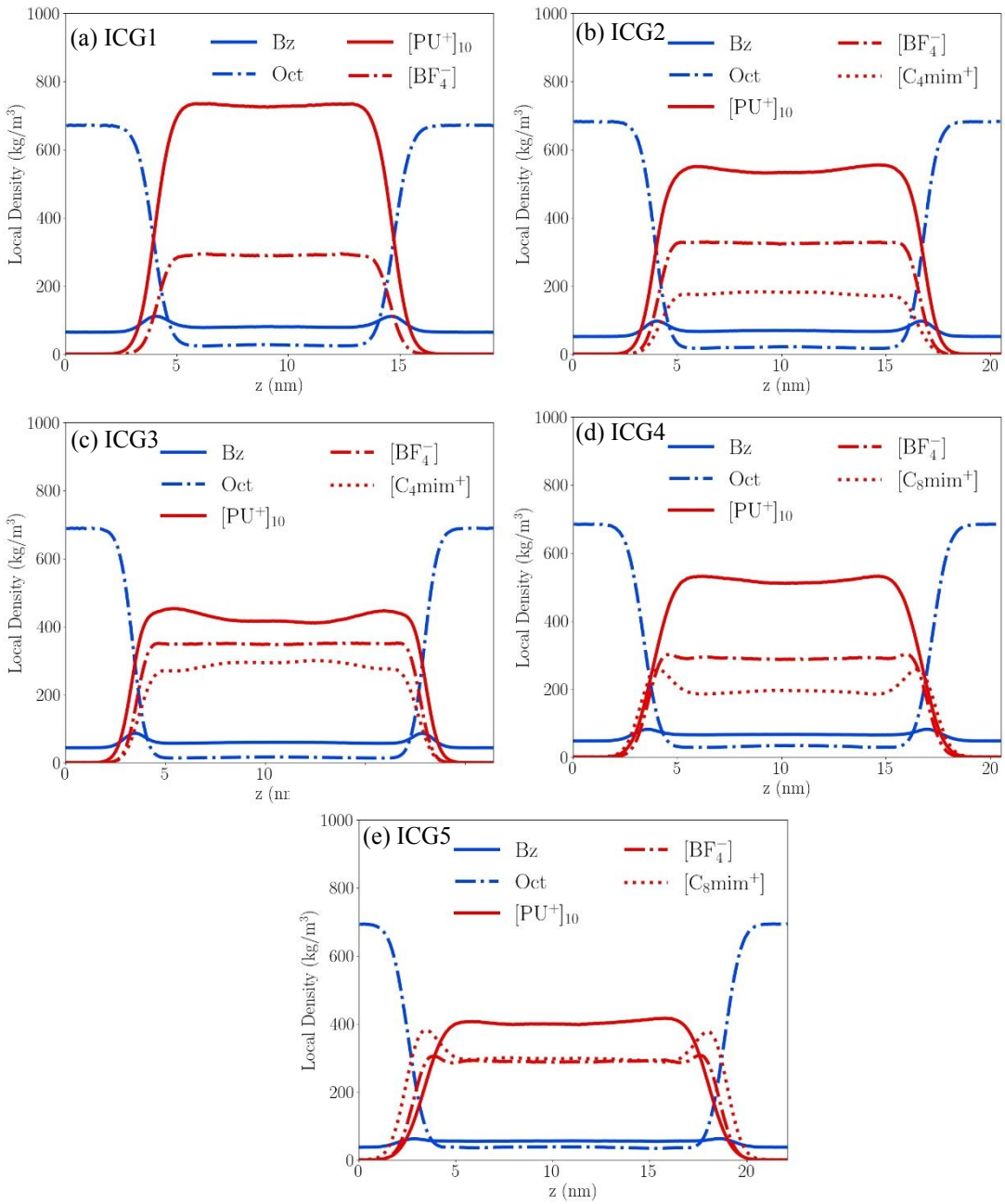


**Figure S3**. Local mass density of the interfacial systems: (a) ICG1, (b) ICG2, (c) ICG3, (d) ICG4, and (e) ICG5 at 348 K and 1 bar.

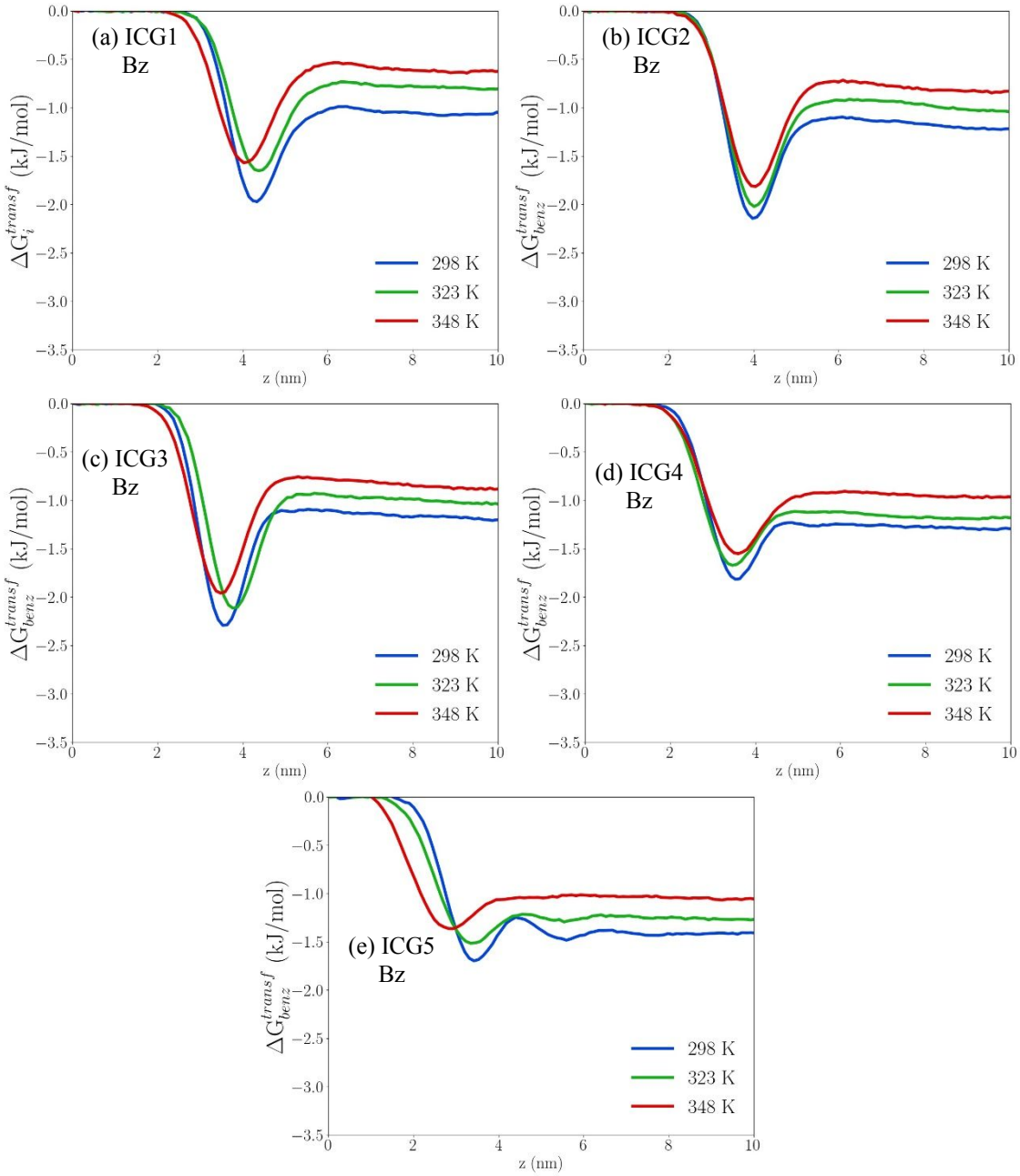


**Figure S4**. Temperature dependence of the free energy profiles of transferring Bz from the oil phase for the interfacial systems: (a) ICG1, (b) ICG2, (c) ICG3, (d) ICG4, and (e) ICG5.

**Table S1.** Distribution coefficient and benzene selectivity.

| System | Temperature (K) | $D_{Oct}$ | $D_{Bz}$ | S |
|---|---|---|---|---|
| ICG1 | 298 | 0.161 | 11.262 | 70.091 |
| | 323 | 0.215 | 9.864 | 45.815 |
| | 348 | 0.271 | 8.539 | 31.494 |
| ICG2 | 298 | 0.152 | 14.230 | 93.640 |
| | 323 | 0.190 | 12.557 | 65.939 |
| | 348 | 0.245 | 10.924 | 44.567 |
| ICG3 | 298 | 0.136 | 16.956 | 124.872 |
| | 323 | 0.180 | 14.912 | 83.039 |
| | 348 | 0.226 | 13.096 | 57.942 |
| ICG4 | 298 | 0.028 | 1.706 | 60.147 |
| | 323 | 0.037 | 1.570 | 42.476 |
| | 348 | 0.048 | 1.413 | 29.504 |
| ICG5 | 298 | 0.314 | 15.688 | 50.040 |
| | 323 | 0.367 | 13.452 | 36.702 |
| | 348 | 0.429 | 11.057 | 25.766 |
| ICG6 | 298 | 0.016 | 11.363 | 725.441 |
| | 323 | 0.027 | 10.492 | 390.829 |
| | 348 | 0.041 | 9.854 | 242.825 |
| ICG7 | 298 | 0.613 | 5.955 | 9.717 |
| | 323 | 0.624 | 5.723 | 9.173 |
| | 348 | 0.660 | 5.138 | 7.783 |