Supporting Information

Capacitive Performance of Amino Acid Ionic Liquid Electrolyte-based Supercapacitors by Molecular Dynamics Simulation

Mingbing Wu,[1,2,3] Wei Li, [1,2,3] Song Li[1,2,3], Guang Feng[1,3]*

[1]State Key Laboratory of Coal Combustion, School of Energy and Power Engineering, Huazhong University of Science and Technology, 430074, China.

[2]Shenzhen Research Institute of Huazhong University of Science and Technology, Shenzhen, 518057, China.

[3]Nano Interface Centre for Energy, School of Energy and Power Engineering, Huazhong University of Science and Technology, 430074, China.

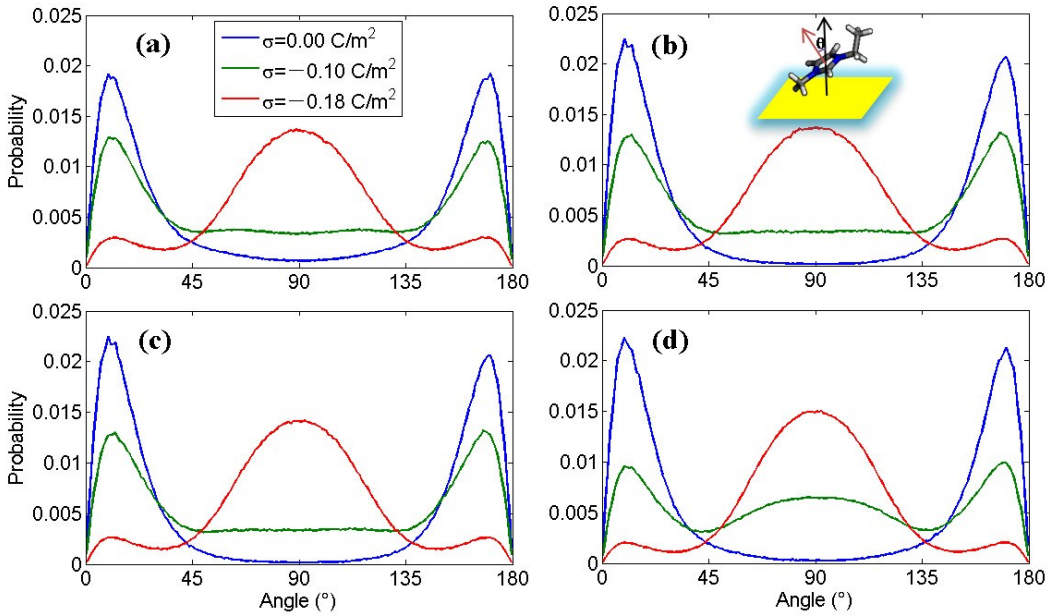

Figure S1. The orientation distribution probability of cation $[EMIM]^+$ of the four types of AAILs(a, b, c and d represent [EMIM][GLY] [EMIM][SER], [EMIM][VAL] and [EMIM][PHE], respectively) across EDLs at varying surface charge densities. The angle is formed between the normal vector of the electrode and the normal vector of imidazole ring of $[EMIM]^+$as the inset shows in panel b. The similar behavior of cation $[EMIM]^+$ in each type of AAIL indicated that different sizes of anions or side chains of anions impose slight effects on the behavior of the common cation.

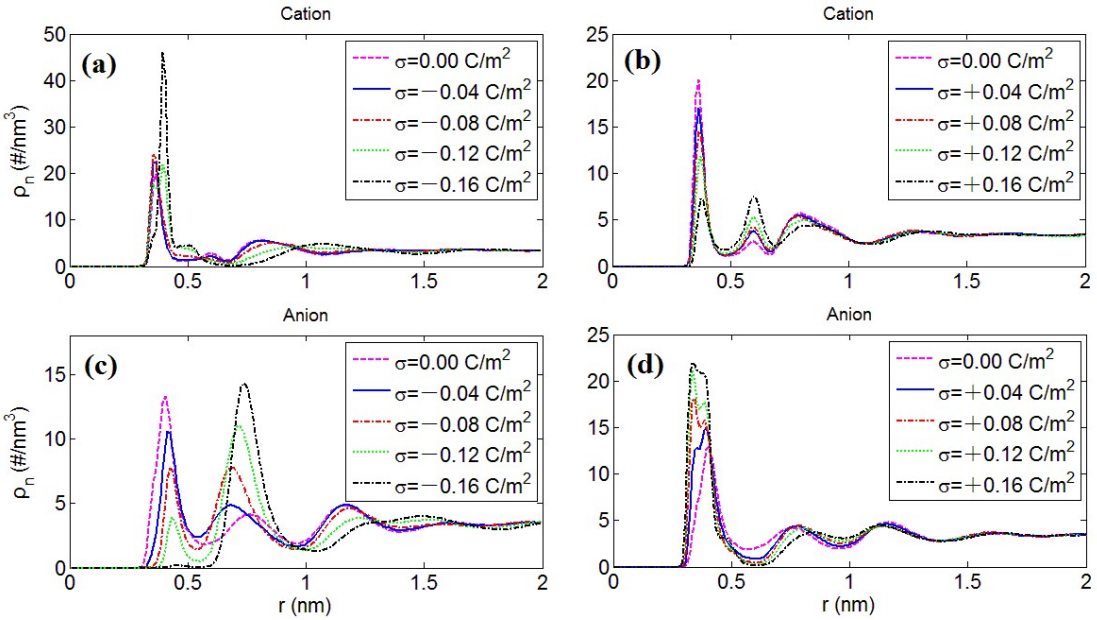

Figure S2. The number density profiles of cation $[EMIM]^+$ (a, b) and anion $[GLY]^-$ (c, d) as a function of distance towards electrode surface at positive or negatively

charged electrode of varying surface charge density.

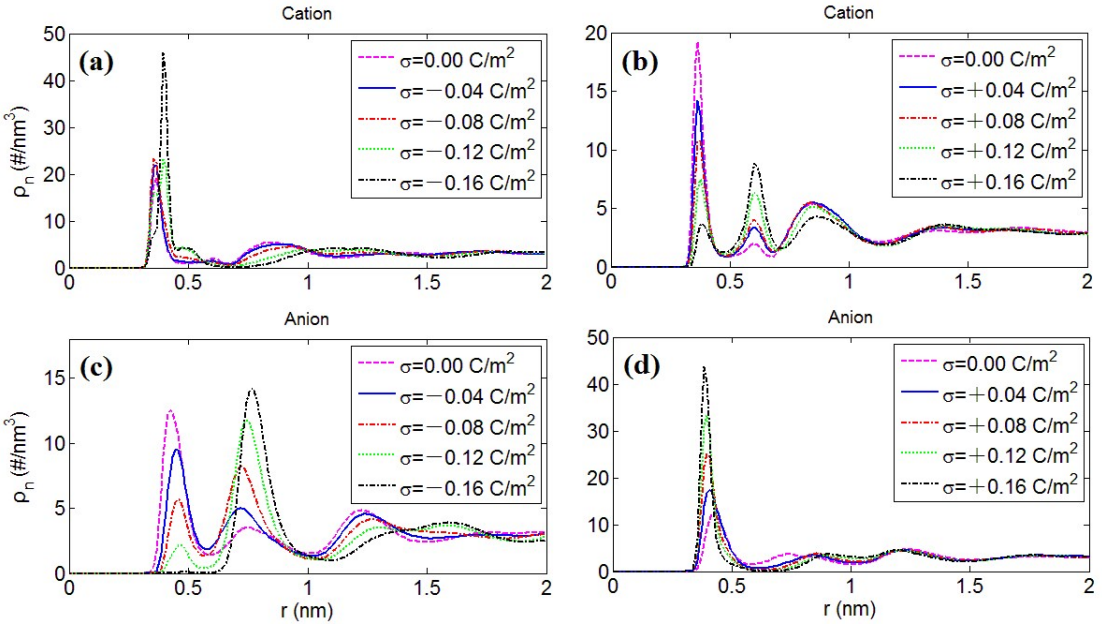

Figure S3. The number density profiles of cation $[EMIM]^+$ (a, b) and anion $[SER]^-$ (c, d) as a function of distance towards electrode surface at positive or negatively charged electrode of varying surface charge density.

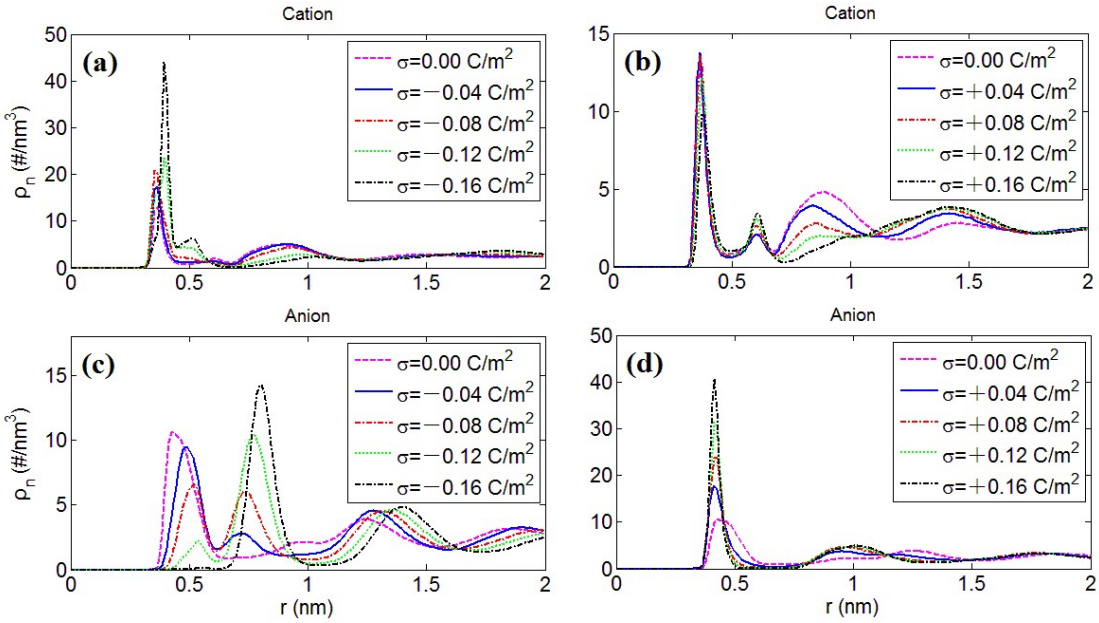

Figure S4. The number density profiles of cation $[EMIM]^+$ (a, b) and anion $[VAL]^-$ (c, d) as a function of distance towards electrode surface at positive or negatively charged electrode of varying surface charge density.

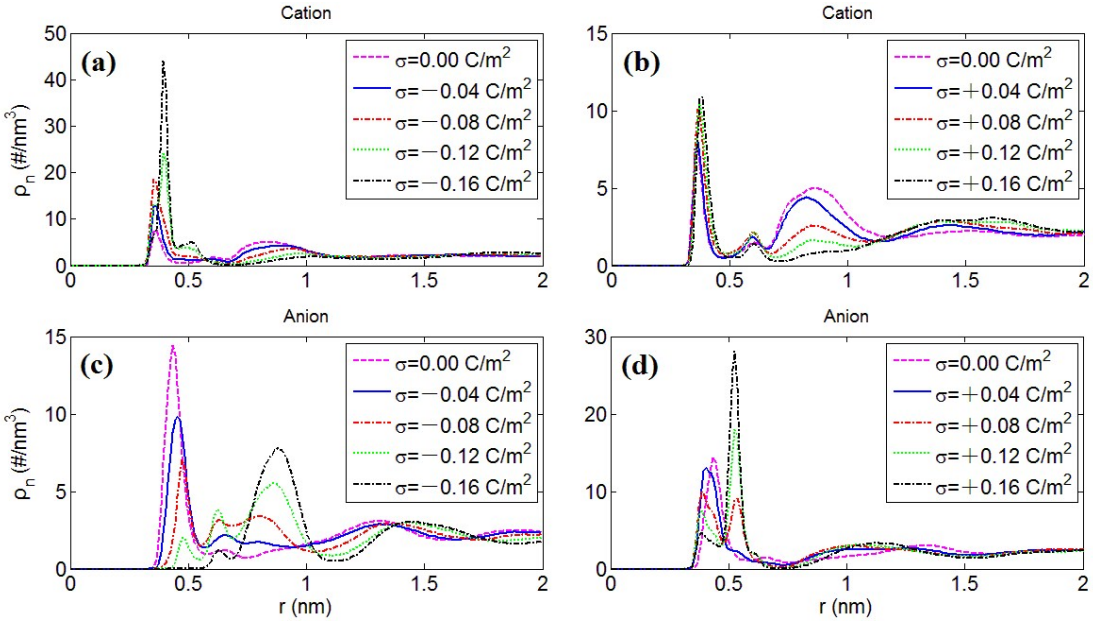

Figure S5. The number density profiles of cation $[EMIM]^+$ (a, b) and anion $[PHE]^-$ (c, d) as a function of distance towards electrode surface at positive or negatively charged electrode of varying surface charge density.