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1. Sigma profiles and sigma potentials

The charge density profiles of the molecular surface are represented by the σ-profile which can be divided into three important sections: hydrogen bond donor for $\sigma < -0.01$ e/Å^2, the non-polar region for $-0.01 < \sigma < +0.01$ e/ Å^2, and hydrogen bond acceptor for $\sigma > +0.01$ e/ Å^2. [1-3]

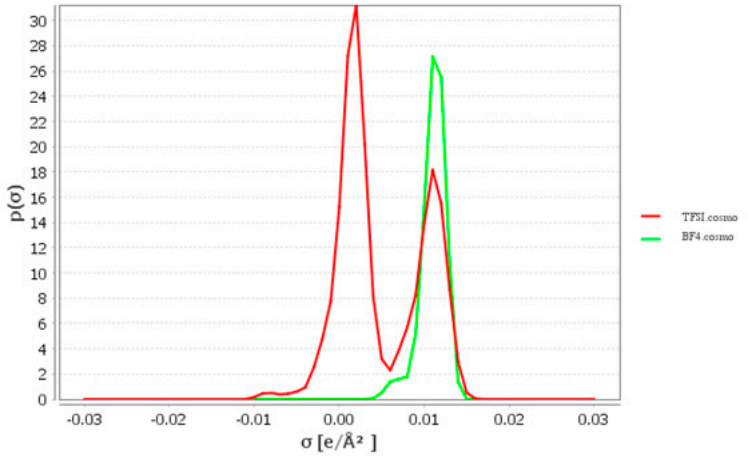

Figure S1: Sigma profile for TFSI and BF_4

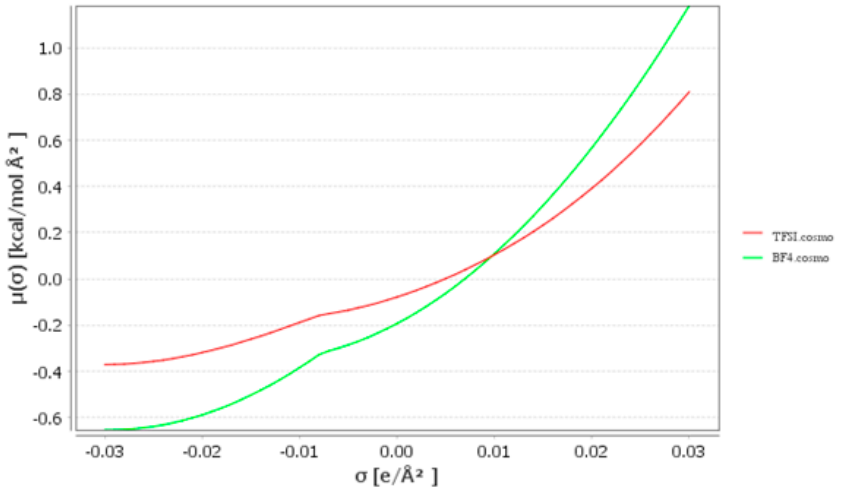

Figure S2: Sigma potential for TFSI and BF_4

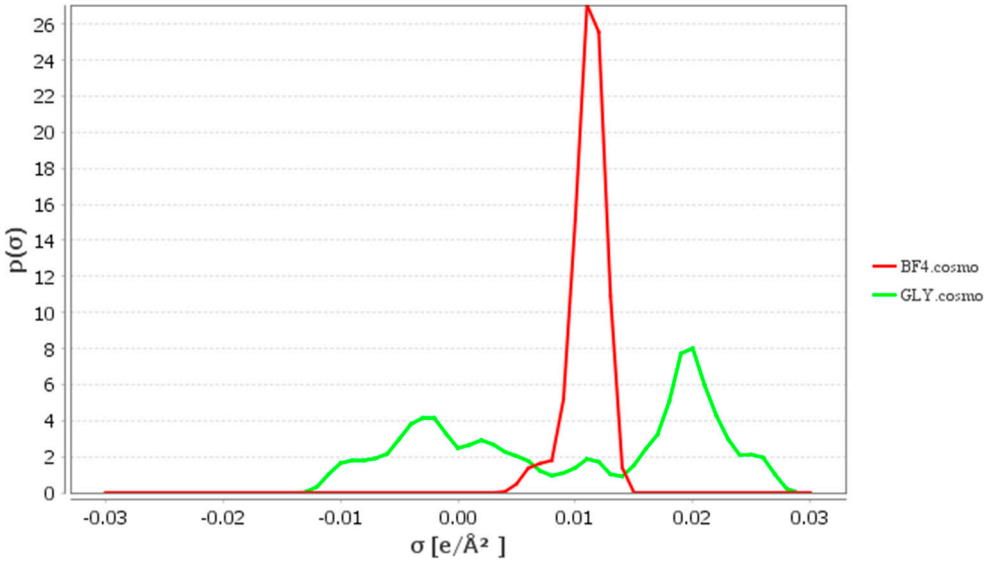

Figure S3: Sigma profile for GLY and BF_4

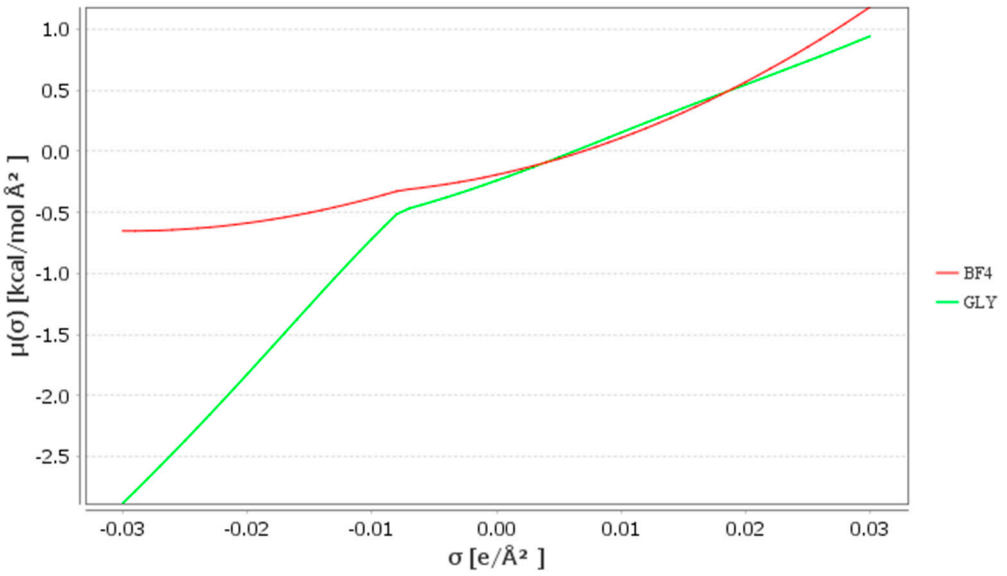

Figure S4: Sigma potential for GLY and BF_4

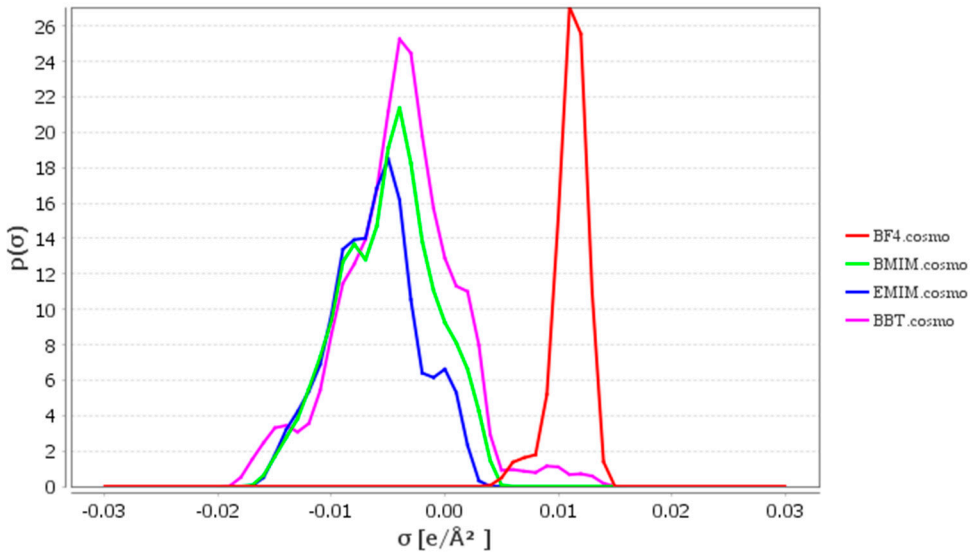

Figure S5: Sigma profiles for EMIM, BMIM, BBT, and BF_4

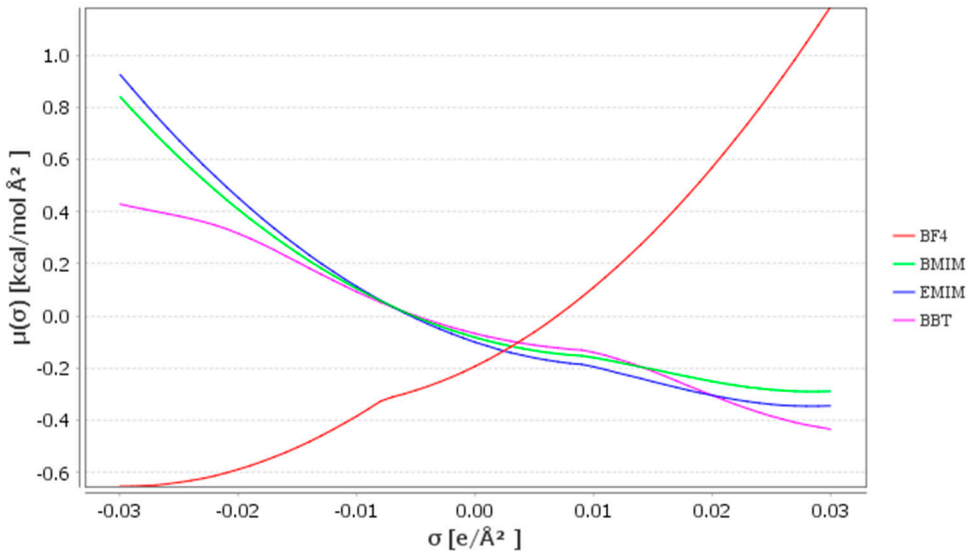

Figure S6: Sigma potentials for EMIM, BMIM, BBT, and BF_4

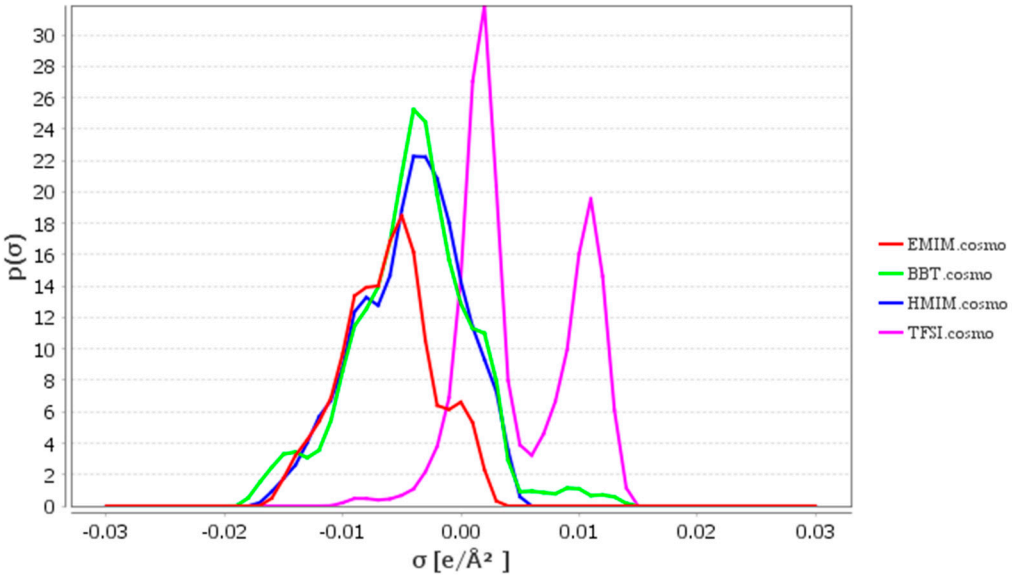

Figure S7: Sigma profiles for EMIM, HMIM, BBT, and TFSI

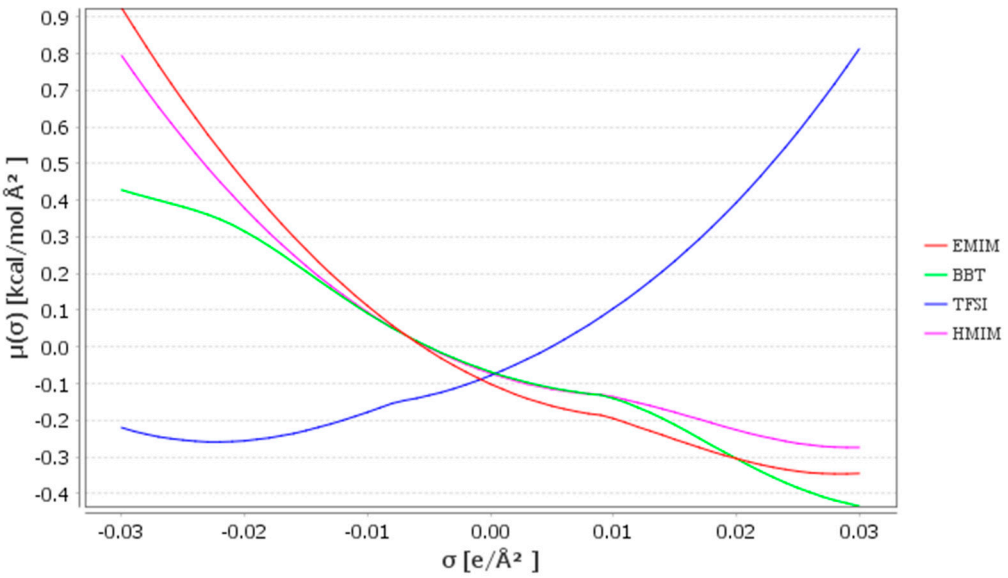

Figure S8: Sigma potentials for EMIM, HMIM, BBT, and TFSI

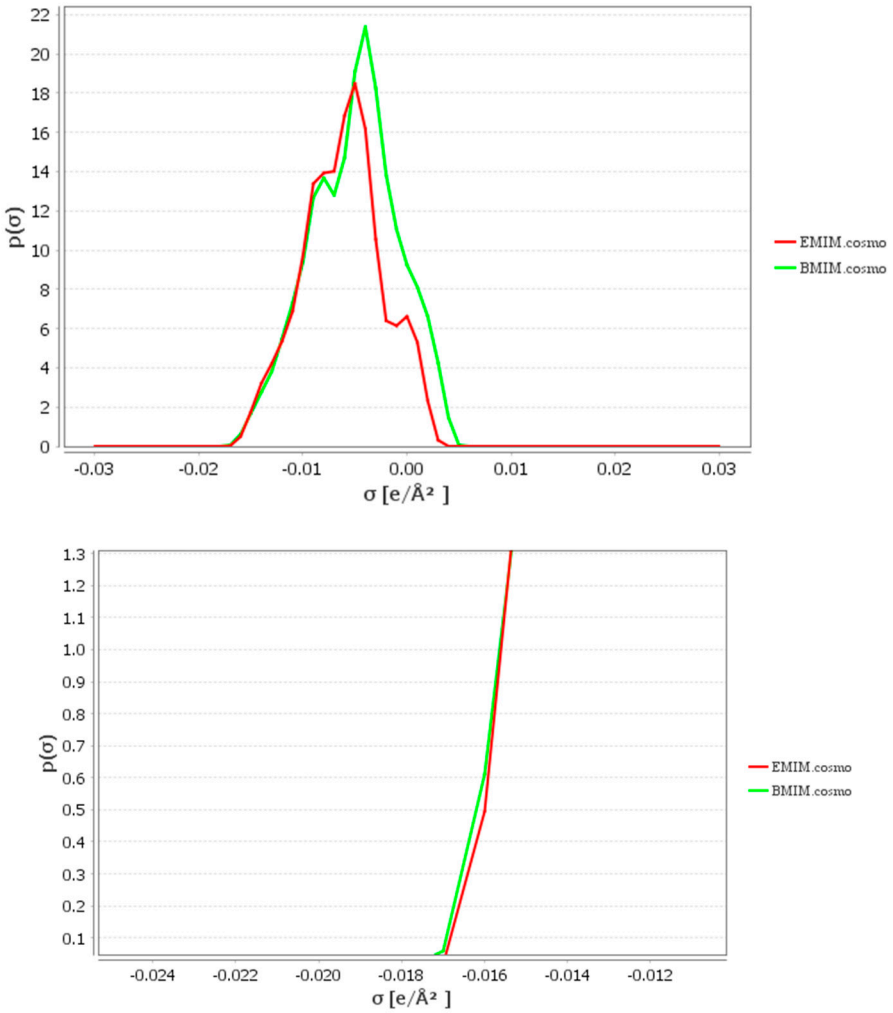

Figure S9: Sigma profiles for EMIM and BMIM (zoom)

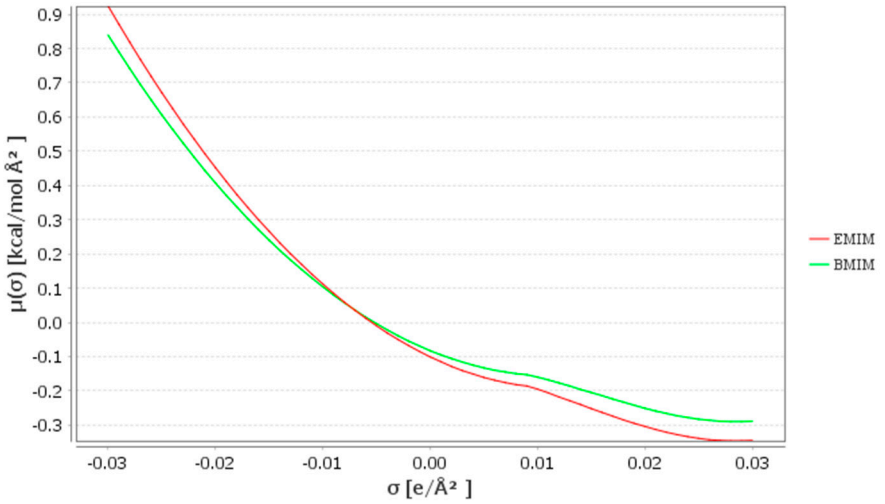

Figure S10: Sigma potentials for EMIM and BMIM

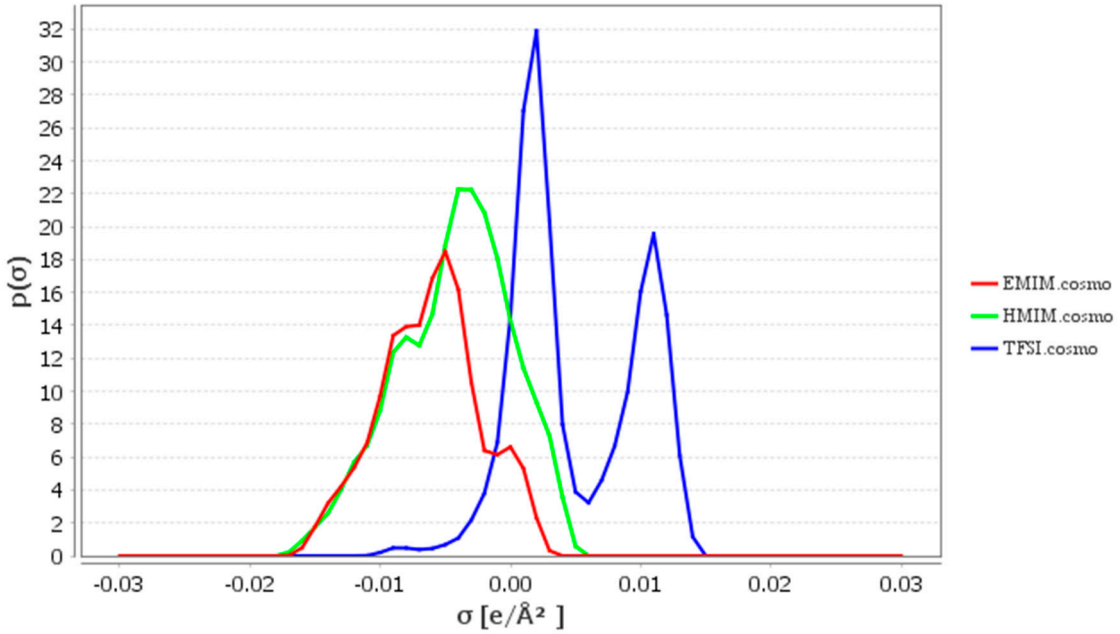

Figure S11: Sigma profiles for EMIM, HMIM and TFSI

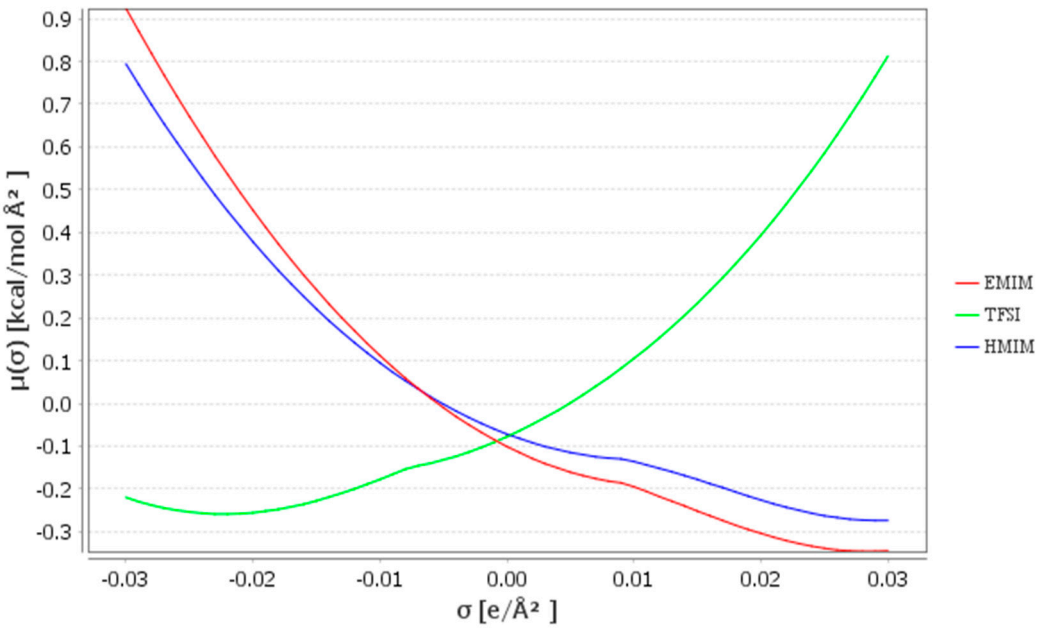

Figure S12: Sigma potentials for EMIM, HMIM and TFSI

2. Sigma surface

The visualization of the charge distribution on the surface can be obtained through sigma surface. The strong electronegativity is represented by the colour red, the positive charge region is represented by the blue colour, the partly negative charge area is represented by the colour yellow, and the neutral nature region is represented by green colour [1-3].

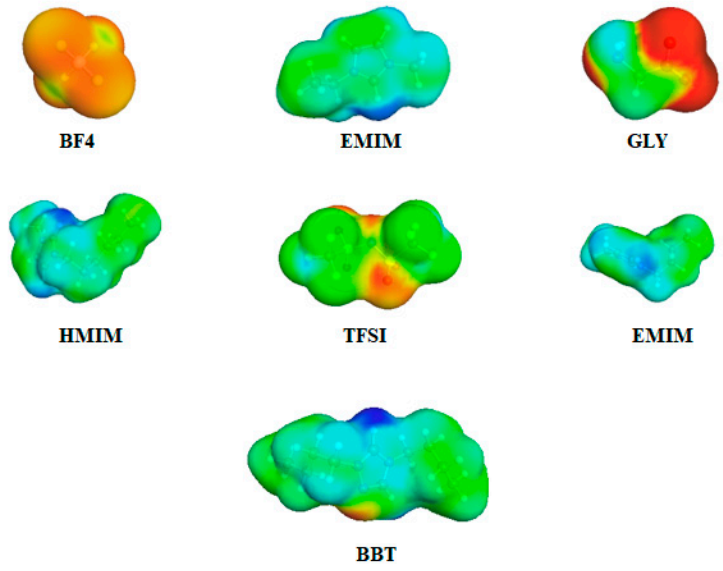

Figure S13: Sigma surface for the chosen cations and anions by employing COSMO-RS

References:

[1] A. Klamt, V. Jonas, T. Bürger, and J. C. Lohrenz, "Refinement and parametrization of COSMO-RS," *J. Phys. Chem A,* vol. 102, no. 26, pp. 5074-5085, 1998.

[2] A. Klamt, "COSMO-RS for aqueous solvation and interfaces," *Fluid Phase Equilib* vol. 407, pp. 152-158, 2016.

[3] A. Klamt, *COSMO-RS: from quantum chemistry to fluid phase thermodynamics and drug design*. Germany: Elsevier, 2005.