Supporting Information

Understanding of Bulk and Interfacial Structures Ternary and Binary Deep Eutectic Solvents with a Constant Potential Method: A Molecular Dynamics Study

Kayvan Moradi ^{a,b,*}, Sirvan Rahimi ^a, Sadollah Ebrahimi ^{b,c,d,*}, Abdollah Salimi ^{a,b,*}

^aDepartment of Chemistry, University of Kurdistan, 66177-15175, Sanandaj, Iran

^bResearch Center for Nanotechnology, University of Kurdistan, 66177-15175, Sanandaj,

Iran

^cDepartment of Physics, Faculty of Science, University of Kurdistan, Sanandaj, Iran

^dLaboratory of Physical Chemistry of Matter (LPCM), Department of chemistry, Université

de Sherbrooke, Sherbrooke, Canada

^{*} Corresponding authors: Tel.: +98 8733624001; fax: +98 87336624008.

E-mail addresses: <u>absalimi@uok.ac.ir</u>, <u>absalimi@yahoo.com</u> (A.Salimi),

E-mail address: kayvan.moradi.1993@gmail.com (K.Moradi),

E-mail addresses: <u>s.ebrahimi@uok.ac.ir</u>, <u>sadollah.ebrahimi@usherbrooke.ca</u> (S.Ebrahimi)

Table S1: The calculated and experimental value of the density of the ternary DES at 300.15 K. The relative percent deviations (Dev%) a between the calculated and experimental value.

Property	Simu.	Exp.	Dev%
Density (gr.cm ⁻³)	1.158	1.136	1.9



Figure S1: Direction vectors were used for the computation of orientational order parameters (a) choline cation and (b) urea.



Figure S2: The electrostatic potential (V) as a function of the distance between graphene sheets (Z) for the two types of supercapacitors investigated. (a) DES-t (b) DES-b