

Supporting Information

Mechanistic Insights into Carbon Dioxide Utilization by Superoxide Ion Generated Electrochemically in Ionic Liquid Electrolyte

Ahmed Halilu^{a, b}, Maan Hayyan^{b, c*}, Mohamed Kheireddine Aroua^{a, d, e*}, Rozita Yusoff^{a*}, Hanee Farzana^a

*^aDepartment of Chemical Engineering, University of Malaya, Kuala Lumpur
50603, Malaysia*

*^bUniversity of Malaya Centre for Ionic Liquids (UMCiL), University of Malaya,
Kuala Lumpur 50603, Malaysia*

*^cChemical Engineering Program, Faculty of Engineering and Technology, Muscat University,
P.O. Box 550, Muscat, P.C. 130, Oman*

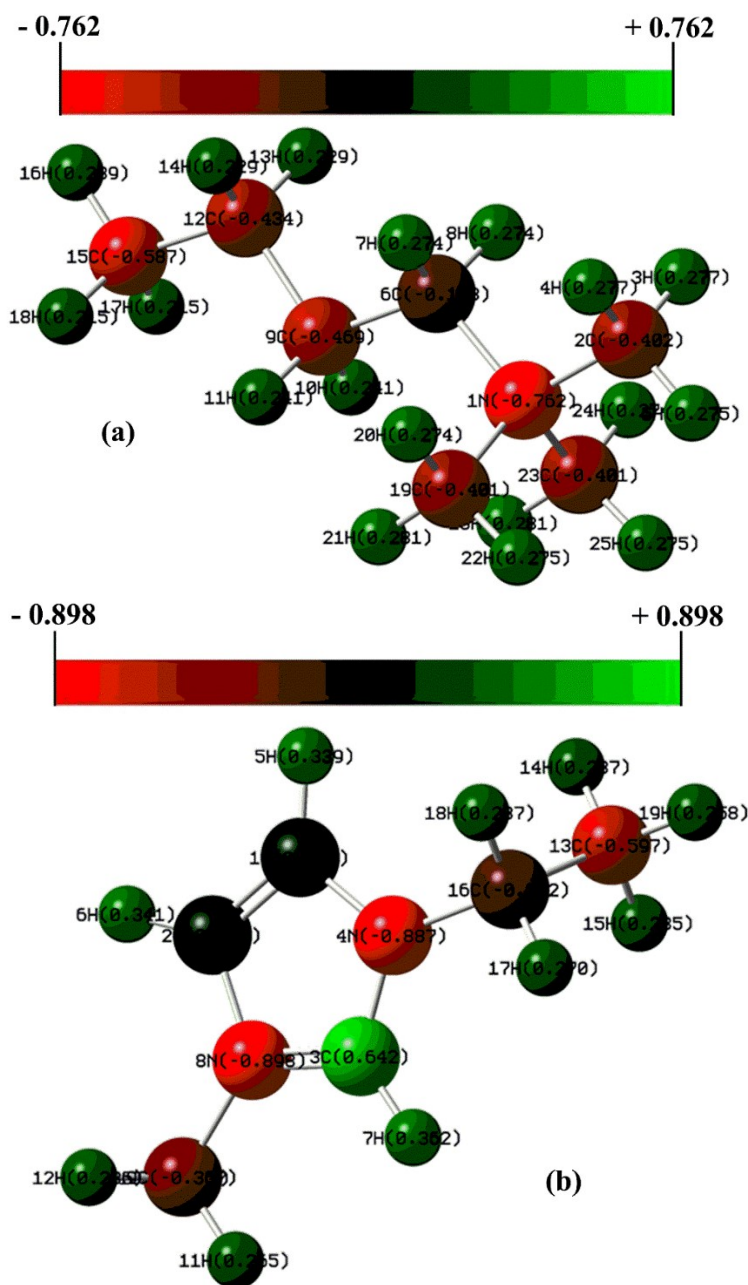
*^dCentre for Carbon Dioxide Capture and Utilization (CCDCU), School of Science and
Technology, Sunway University, Bandar Sunway, 47500 Petaling Jaya, Malaysia*

^eDepartment of Engineering, Lancaster University, Lancaster, LA1 4YW, UK

Email Addresses: maan_hayyan@yahoo.com (M. Hayyan); kheireddinea@sunway.edu.my
(M.K. Aroua); ryusoff@um.edu.my (R. Yusoff)

Table S1: Evidence of irreversibility of $O_2^{\bullet -}/O_2$ using peak separation E_p^c and $E_{p/2}^c$.

ILs	$ E_p^c - E_{p/2}^c $					
	9 mV/s	36 mV/s	64 mV/s	81 mV/s	100 mV/s	144 mV/s
[BMAm ⁺][TFSI ⁻]	89.100	101.400	83.400	85.400	87.500	85.400
[EMIm ⁺][TFSI ⁻]	138.900	135.900	104.500	97.000	95.600	92.400



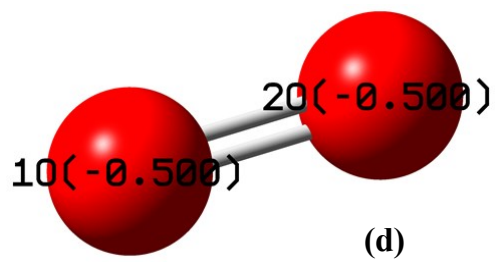
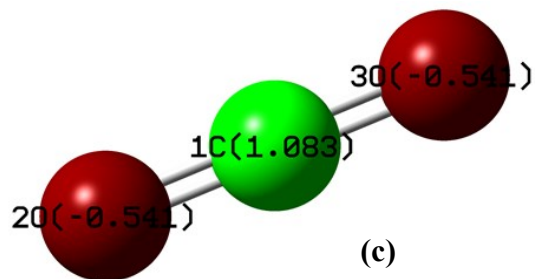


Figure S1: Mulliken atomic charges for (a) [BMAm⁺], (b) [EMIm⁺], (c) CO₂ and (d) O₂^{•-} at Hartree-fock/3-21G level of theory, singlet spin.

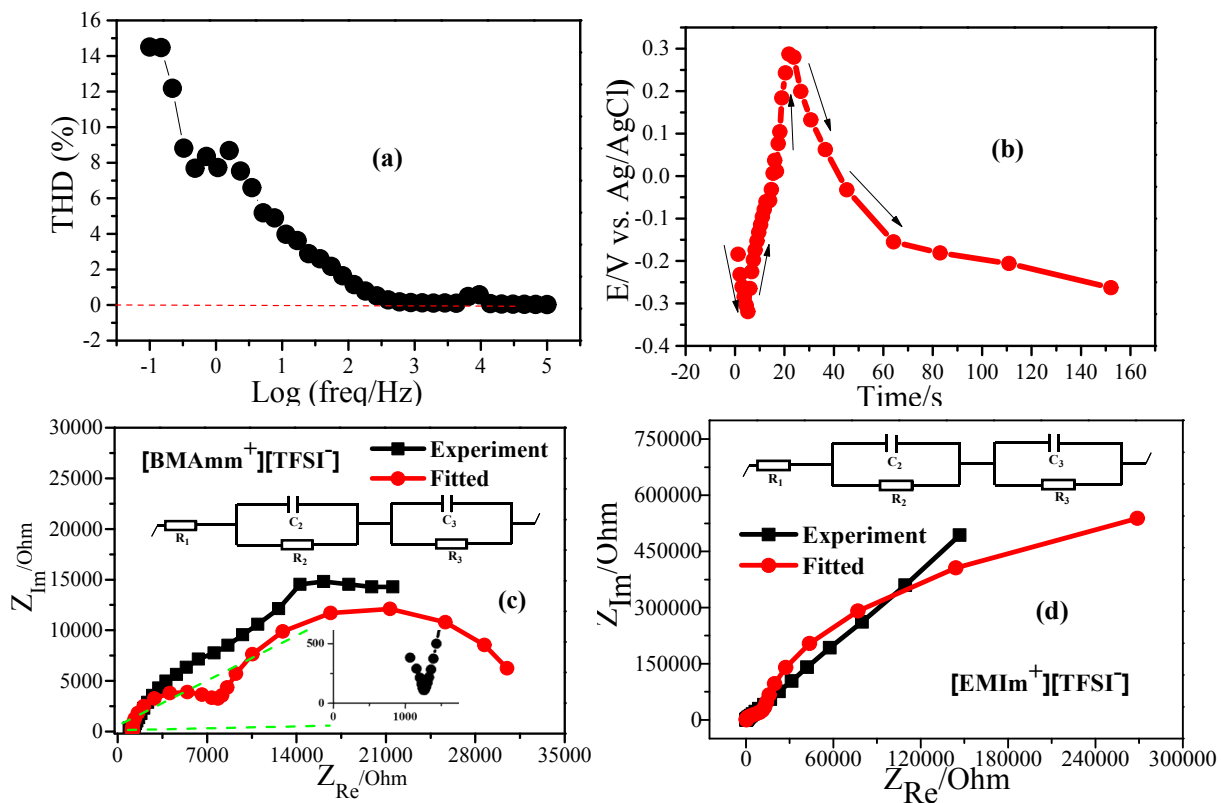


Figure S2: (a) Total harmonic distortion in [BMImm⁺][TFSI⁻] medium (b) Sinusoid of voltage flow in [BMImm⁺][TFSI⁻] medium (c) Nyquist plot of [BMImm⁺][TFSI⁻] medium (d) Nyquist plot of [EMIm⁺][TFSI⁻] medium.