World Academy of Science, Engineering and Technology
International Journal of Chemical and Molecular Engineering
Vol:10, No:03, 2016

DFT Theoretical Investigation for Evaluating Global Scalar Properties and Validating with Quantum Chemical Based COSMO-RS Theory for Dissolution of Bituminous and Anthracite Coal in Ionic Liquid

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Abstract : Global scalar properties are calculated based on higher occupied molecular orbital (HOMO) and lower unoccupied molecular orbital (LUMO) energy to study the interaction between ionic liquids with Bituminous and Anthracite coal using density function theory (DFT) method. B3LYP/6-31G* calculation predicts HOMO-LUMO energy gap, electronegativity, global hardness, global softness, chemical potential and global softness for individual compounds with their clusters. HOMO-LUMO interaction, electron delocalization, electron donating and accepting is the main source of attraction between individual compounds with their complexes. Cation used in this study: 1-butyl-1-methylpyrrolidinium [BMPYR], 1-methyl -3-propylimmidazolium [MPIM], Tributylmethylammonium [TMA] and Tributylmethylphosphonium [MTBP] with the combination of anion: bis(trifluromethylsulfonyl)imide [Tf2N], methyl carbonate [CH3CO3], dicyanamide [N(CN)2] and methylsulfate [MESO4]. Basically three-tier approach comprising HOMO/LUMO energy, Scalar quantity and infinite dilution activity coefficient (IDAC) by sigma profile generation with COSMO-RS (Conductor like screening model for real solvent) model was chosen for simultaneous interaction. [BMPYR]CH3CO3] (1-butyl-1-methylpyrrolidinium methyl carbonate) and [MPIM][CH3CO3] (1-methyl -3-propylimmidazolium methyl carbonate) are the best effective ILs on the basis of HOMO-LUMO band gap for Anthracite and Bituminous coal respectively and the corresponding band gap is 0.10137 hartree for Anthracite coal and 0.12485 hartree for Bituminous coal. Further ionic liquids are screened quantitatively with all the scalar parameters and got the same result based on CH-π interaction which is found for HOMO-LUMO gap. To check our findings IDAC were predicted using quantum chemical based COSMO-RS methodology which gave the same trend as observed our scalar quantity calculation. Thereafter a qualitative measurement is doing by sigma profile analysis which gives complementary behavior between IL and coal that means highly miscible with each other.

Keywords : coal-ionic liquids cluster, COSMO-RS, DFT method, HOMO-LUMO interaction
Conference Title : ICCME 2016 : International Conference on Chemical and Molecular Engineering
Conference Location : Rome, Italy
Conference Dates : March 21-22, 2016