

Amino Acid Functionalized Imidazolium-based Ionic Liquids for CO₂ Capture—A Theoretical and Experimental Approach

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1-methyl-3-ethyl-imidazolium based amino acid ionic liquid [(EMIM)AA]-IL supported on ordered mesoporous silica i.e. SBA-15, was synthesized via grafting method for CO₂ absorption-desorption. Four different kinds of amino-acids (AA) [lysine (Lys), glycine (Gly), alanine (Ala), proline (Pro)] were selected to evaluate their performance. The CO₂ adsorption-desorption studies are carried out using thermogravimetric analysis based on the weight changes. The DFT calculations were carried out for all the aforementioned amine functionalized ionic liquids to investigate the structural deformation and binding energetics between CO₂ and various ionic liquids in atomic scale. We found that the energy required for CO₂ adsorption on lysine (-0.98 eV) shows the high enough for CO₂ uptake. Moreover, OMS-IL(Lys) shows the better performance at 25 °C obtained from the CO₂-TGA experiments, which is in good agreement with the DFT calculation. This work was supported by KCRC through the NRF funded by Ministry of Science, ICT, and Future Planning (NRF-2014M1A8A1049258).