MOLECULAR SIMULATION OF IONIC LIQUIDS AND IONIC LIQUID-POLYMER HYBRID SYSTEMS

M. Panou[1], K. Karanasiou[1], A. Argyropoulou[1], N. Vergadou[1,*]

[1] Institute of Nanoscience and Nanotechnology, NCSR "Demokritos", Athens, Greece

(n.vergadou@inn.demokritos.gr)*

ABSTRACT

Ionic Liquids (ILs) are a rapidly growing class of materials with a broad spectrum of applications that range from green chemistry, catalysis, biotechnology, food, and medical industry to separation technologies and environmental engineering. ILs are organic salts that are in the liquid state at room temperature and by convention below 100°C. They exhibit a unique combination of properties [1] such as extremely low vapor pressures, thermal stability, chemical tunability, good electrolytic, separation and solvation properties, non-flammability and easy recycling. The combination of these properties renders them ideal for use in a plethora of industrial applications [2] such as solvents and catalysts in synthesis, as lubricants, as electrolytes in electrochemistry and in gas storage and CO_2 capture applications [3,4]. The organic and simultaneously ionic nature of the constitutive ions results in diverse interactions that directly affect the microscopic structure and the dynamical behaviour of ILs. Simultaneously, the need to develop new high performance functional materials necessitates the exploration and development of new cutting-edge composites and to unravel the molecular mechanisms and microscopic characteristics that govern their macroscopic properties. Molecular simulation methods are proven to be an extremely valuable means of reliable property prediction, enabling simultaneously the elucidation of the underlying mechanisms that are responsible for the macroscopic behavior of materials.

The present work focuses on the molecular simulation of imidazolium-based [TCM^-] ionic liquids using an optimized and validated classical atomistic force field [5,6]. Molecular simulations have been applied at various thermodynamic conditions and also in mixtures with CO_2 up to high pressures. A wide range of properties such thermodynamic, structural, dynamics and transport properties have been calculated and the effect of CO_2 concentration and of temperature on the above properties has been thoroughly investigated. Sorption isotherms and associated volumetric effects have been extracted using a multistage iterative scheme[7]. Molecular simulation methodologies were also implemented for the study of ILs/PVDF polymer hybrid systems and the microscopic mechanisms that are responsible for the behavior of composite materials were thoroughly investigated.

KEYWORDS: molecular simulation, ionic liquids, composites, microscopic mechanisms, properties prediction

REFERENCES

[1] Rogers R. D., Seddon K. R. (2003). *Science*, 302, no. 5646, 792–793.

[2] Wasserscheid P., Welton T. (eds.) (2003). Ionic Liquids in Synthesis, Wiley-VCH: Weinheim, Germany.

[3] Vergadou N., Androulaki E., I. G. Economou (2017). Molecular Simulation Methods for CO_2 Capture and Gas Separation with Emphasis on Ionic Liquids, in Process Systems and Materials for CO_2 Capture: Modelling, Design, Control and Integration (eds A. I. Papadopoulos and P. Seferlis), John Wiley & Sons, Ltd, Chichester, UK.

[4] Romanos G., Vergadou N., I.G. Economou (2022). "Ionic Liquids in Carbon Capture" in Sustainable Carbon Capture: Technologies and Applications, Suleman, H., Fosbøl, P.L., Nasir, R., & Ameen, M. (Eds.), CRC Press.

[5] Vergadou N., E. Androulaki, Hill J.-R., Economou I.G. (2016) *Phys. Chem. Chem. Phys.*, 18, 6850-6860.

[6] Zubeir L.F., Rocha M.A.A., Vergadou N., Weggemans W.M.A., Peristeras L.D., Schulz P.S., Economou I.G., M.C. Kroon (2016). *Phys. Chem. Chem. Phys.,* 18, 23121-23138.

[7] Ricci E., Vergadou N., Vogiatzis G.G., De Angelis M.G., Theodorou D.N. (2020). *Macromolecules*, 53, 3669-3689.