Ionic liquids (ILs) are organic salts that are in liquid state near room temperature. ILs have been proposed as alternative electrolytes for energy storage in electrochemical double-layer capacitors (EDLCs). These devices have a structure similar to a battery, consisting of two carbon-based nanoporous electrodes, an electrolyte and an ion-permeable separator. Furthermore, inserting organic salts inside nm-sized cylindrical pores is one step in the synthesis of optically-active and magnetic 1D-nanostructures (nanorods, nanowires, nanotubes) based on organic salts. These IL-based nanomaterials hold promise for potential applications in biomedicine (e.g., magnetic hyperthermia cancer treatment, medical imaging), optics and photovoltaics.

A fundamental understanding of the behavior of organic salts inside nm-sized pores is crucial to optimize the applications mentioned above, as relevant macroscopic properties of these systems (e.g., electrical capacitance and resistance, and magnetic and optical properties) typically depend on the molecular-level properties of the confined ILs. Here we report classical molecular dynamics (MD) simulations of typical ILs, such as \([\text{bmim}^+][\text{PF}_6^-]\) and \([\text{dmim}^+][\text{Cl}^-]\), confined inside carbon materials with nanopores of different sizes and geometries (namely carbon nanotubes, graphitic slit-like pores, and ordered mesoporous carbons such as CMK-3). Our results indicate that variables such as pore size, pore geometry, pore surface roughness and pore loading have a profound influence on the structure and dynamics of confined ILs. The effects of these variables on different properties of the confined ILs (e.g., local density, orientational profiles, radial distribution functions, mean square displacements) will be analyzed and discussed.

Francisco Hung is currently an Assistant Professor and Cain Professor in the Cain Department of Chemical Engineering at Louisiana State University. He has an undergraduate degree in Chemical Engineering from Universidad Simón Bolívar in Caracas, Venezuela, and a master’s degree from the same university. Afterwards, he came to the US and did his PhD in Chemical Engineering at North Carolina State University under the direction of Professor Keith Gubbins. He then worked as a postdoctoral researcher in the Department of Chemical and Biological Engineering at the University of Wisconsin-Madison, in the group of Professor Juan de Pablo. He joined the faculty at LSU in Fall 2007.