ICCRAM Scientific Conference Series on
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"Developing Carbon Capture Technologies Using Computational Chemistry: The Case of Deep Eutectic Solvents"

The control of greenhouse gases in the atmosphere requires the development of suitable CO2 capture technologies for developing sustainable energy production from fossil-fueled power plants. The design of new materials for carbon capture purposes has emerged as key research line these last years, leading to many proposed alternatives with variable degree of success. Among the plethora of considered CO2 sorbents, deep eutectic solvents (DES) have started to attract large attention in the industry and academia because of DES production from low cost and natural sources, null toxicity and total biodegradability. DES are developed from the combination of an hydrogen bond acceptor (HBA), usually a salt, and an hydrogen bond donor (HBD) molecule, which at suitable concentrations leads to an eutectic mixture liquid at ambient temperature. Therefore, millions of DES sorbents can be developed through HBA-HBD-composition combinations, and thus, DES are a large platform for developing gas separation solvents. The huge number of possible DES is one side an advantage, because it allows fine tuning of the physicochemical properties and CO2 solubility, but it is also a problem for developing experimental studies. In this framework, computational chemistry may have a pivotal role for developing DES-based carbon capture technologies. Theoretical studies allow predicting and studying physicochemical properties of large number of DES for developing structure-property relationships, leading to the most suitable HBA-HBD-concentration combinations. Likewise, computational studies allow obtaining a nanoscopic vision of the DES main properties regarding to CO2 capture, which will guide the process of designing the most suitable DES gas sorbents. In this communication, the state-of-the-art on the use of computational methods based on Density Functional Theory and Molecular Dynamics for studying DES - CO2 properties are analyzed, showing the most relevant results and future directions.

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Santiago Aparicio obtained his Ph.D. degree in physical chemistry from the University of Burgos, Burgos, Spain, in 2001. Between 2005 and 2006, he served as a Fulbright Visiting Scholar at the Department of Chemical Engineering, Texas A&M University, College Station, TX, USA. Since 2009, he has worked as a Professor at the Department of Chemistry in the University of Burgos, Spain. His research interests include thermophysical and molecular modeling studies for the characterization and development of new materials in the fields of energy and environment, including ionic liquids, green solvents, metal - organic frameworks, carbon nanosystems, and natural gas hydrates. He has published 130 papers in refereed journals and several book chapters. He is Editor-in-chief of Physical Chemistry Journal and member of the Editorial Board of several journals.

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