COSMO-RS Prediction of Silicon Extraction from Lunar Regolith by Deep Eutectic Solvents

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Abstract

There have been increasing efforts to build a settlement on the Moon in recent years. Developing an in-situ resource utilization becomes significantly essential to generate consumables for a long-term, sustainable, and autonomous human presence in space. Building a self-sufficient civilization requires harnessing resources available on the Moon to produce energy. Approximately 48% of Lunar regolith is made up of silica (SiO_2). Abundant SiO_2 in the Lunar regolith can be utilized in solar cells to produce electricity from sunlight on the Moon. It is vital to use a sustainable, environmentally friendly, and efficient technology to extract SiO_2 from the regolith. Deep eutectic solvents (DESs) have gained attentions in recent years since they are considered environmentally friendly alternatives to typical organic solvents. DESs are often made of eutectic combinations of Lewis or Bronsted acids and bases, and consist of a hydrogen bond acceptor (HBA) and a hydrogen bond donor (HBD). The benefits and features of DESs have been thoroughly reported, including low costs, ease of preparation, low melting point, and negligible vapor pressure. In addition, DESs have other advantages such as non-combustibility, high conductivity, excellent stability, bio-renewability, and biodegradability. Because of the complexity and diversity of DES composition, screening DESs with the best dissolvability is a difficult task. COnductor like Screening MOdel for Real Solvents (COSMO-RS), a model that combines electrostatic theory and statistical thermodynamics, was used to predict the dissolution capacities of SiO_2 in DESs. COSMO-RS calculates the chemical potential of molecules in a liquid solution to determine thermodynamic characteristics such as solubility coefficient and activity coefficient (γ). Using COSMO-RS, the dissolution capacities of SiO_2 in 108 DESs based on 15 HBDs and 29 HBAs were determined. The top 5 DESs for SiO_2 extraction were identified and will be further tested experimentally with Lunar regolith simulants. These DESs are tetraoctylammonium chloride, menthol, thymol, choline chloride, methyl-trioctyl-ammonium chloride, tetra-n-butylammonium chloride, tetra-n-butylammonium hydrogen sulfate, tetraoctylammonium bromide, glycol, lactic acid, decanoic acid, acetic acid, pyruvic acid, caprylic acid, 4-oxo-pentanoicacid, dodecanoic acid, butyric acid, nonanoic acid, 1-decanol, and hexafluoro-i-propanol.