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

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Introduction

- Around half of lunar regolith is made up of silica (SiO_2) (Fig. 1).
- Silicon is used in solar cells to convert light to electricity (Fig. 2).
- Electrochemical methods, molten oxide electrolysis, and microbes have been used to extract silica from lunar regolith (Fig. 3).
- Deep eutectic solvents (DES) are highly tunable solvents that have exceptional ability to dissolve a broad range of compounds, are environmentally friendly, and possess advantageous physicochemical properties (Fig. 4).
- Each DES consists of a pair of hydrogen bond donor (HBD) and hydrogen bond acceptor (HBA). DES are potentially green solvents for mineral extraction from lunar regolith.
- COSMO-RS (COnductor like Screening MOdel for Real Solvents) is a quantum chemistry-based equilibrium thermodynamics method capable of predicting chemical potentials in liquids.
- The solubility of SiO_2 in 108 DES based on 15 HBD and 29 HBA was predicted.

Figure 1. A sample of Lunar regolith simulant.

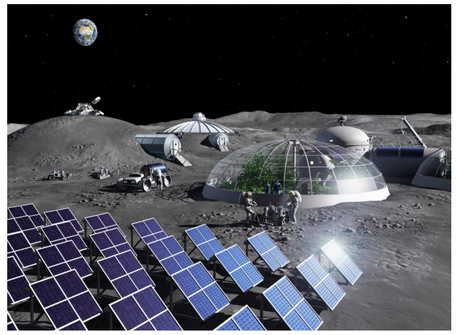

Figure 2. Futuristic impression of human establishment on the Moon. https://spacesettlementprogress.com/lunar-regolith-beneficiation-a-review-of-the-latest-research/

Figure 3. A hydrophobic deep eutectic solvent. https://extractionmagazine.com/2019/10/19/deep-eutectic-solvents/

Figure 4. Chemical structure of SiO_2. https://molview.org

Objectives

- Screen DES for complete dissolution of silica in Lunar regolith.
- Identify top 5 DES for silica extraction experiment.
- Evaluate the selectivity and capacity of task specific DES.
- Investigate optimal conditions for extracting silica from Lunar regolith by selected DES.

Materials and methods

- Thermodynamic properties prediction was executed by COSMO-RS to obtain the capacities of various DES for SiO_2 extraction by calculating ln(γ) (indirect measure of SiO2 solubility).
- COSMO-RS was used as a theoretical basis for the DES selection (Fig. 5).
- Discrete molecular surface to predict thermodynamic properties was created.
- Each formed surface segment was characterized by its surface area and shielding density charge.
- The DESs components in this study were obtained from the COSMOtherm software database.

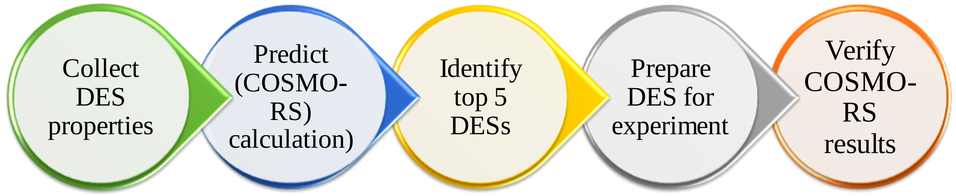

Figure 5. Flowchart of the research process

Key results

- Top 5 DESs in SiO_2 extraction were identified (Table 1).
- The predicted dissolution efficiency in DESs is highly dependent on HBDs.

Table 1. Top 5 potential DES for extracting silica predicted by COSMO-RS

Compounds		ln(γ)	γ quat / tertiary	γ binary	Capacity
HBA	HBD	SiO_2	SiO_2	SiO_2	SiO_2
Choline Chloride	Acetic acid	-0.64	0.52	0.13	7.60
Choline Chloride	4-oxo-pentanoicacid	-0.58	0.56	0.14	7.13
Tetra-n-butylammonium chloride	Acetic acid	-0.79	0.45	0.11	8.85
Tetra-n-butylammonium chloride	4-oxo-pentanoicacid	-0.66	0.51	0.13	7.78
Thymol	Hexafluoro-i-propanol	-1.53	0.21	0.11	9.25

Key results (continued)

- Thymol had the highest predicted SiO_2 extraction with hexafluoro-*i*-propanol.
- Prediction SiO_2 extraction capacity by thymol (HBA), with other HBDs was poor (< 1.0).
- Tetra-*n*-butylammonium chloride (HBA) had the highest average SiO_2 predicted extraction capacity with other HBDs (Capacity = 5.0).
- The capacity of tetra-n-butylammonium chloride with other HBDs were evaluated for SiO_2 extraction (Table 2).

Table 2. Activity coefficients of tetra-*n*-butylammonium chloride with other HBDs.

No	Compound	ln(γ)
1	SiO_2	-0.47
2	Tetra-n-butylammonium	0.0
3	Cl_anion	0.0
4	Lactic acid	-5.27
5	Acetic acid	-3.49
6	Pyruvic acid	-4.02
7	Caprylic acid	-3.14
8	Butyric acid	-3.56
9	Nonanoic acid	-3.00
10	Hexafluoro-i-propanol	-9.35

Conclusions

- COSMO-RS can be used to screen DESs for extracting SiO_2 from Lunar regolith.
- Certain DES have high capacities for SiO_2.
- Analysis of activity coefficients suggests that hydrogen bonds are the primary contributor to DES's ability to extract SiO_2.

Future work

- Experimentally evaluate the capacity of the top 5 DES and identify the best performing DES in extraction of SiO_2.

Acknowledgement

- The project is funded by the 2021-2022 NV NASA EPSCoR RID Seed Grant.