Contribution ID: **5** Type: **Student Micro-talk**

DFT Modelled Deep Eutectic Solvent (DES) – Pyrite interactions

In this work Kohn-Sham density functional theory (KS-DFT) calculations have been used to get a better understanding of the re-mining efforts of pyrite and tailings. In refractory ores the precious metal gold occurs as micro/nano-inclusion encapsulated within the crystal lattice of host mineral pyrite (FeS2). Therefore, the encapsulated gold is inaccessible to the reagent for extraction. Since the gold is locked inside the sulfidic host mineral, it is necessary to break down the matrix to expose the encapsulated gold. One of the latest ways to do this is using deep eutectic solvent (DES) in which the host mineral (FeS2) is electrochemically oxidised/dissolved in a DES medium, to make the gold accessible for extraction. The specific DES used is a (1:2) molar ratio of choline chloride (ChCl) and ethylene glycol (EG). There are two ligands available in (1ChCl:2EG) DES, Cl– and EG as O-donor chelating ligand to react with the iron. To determine whether Cl– or EG will from the most stable complex with Fe2+or Fe3+, DFT calculations were conducted using the High Performance Computing (HPC) facilities of the CHPC in South Africa.
FeS2 ⟶ Fe2+/ Fe3+ + Sx2– ⟶ SO42– + S0 Cl– EG2–
[Fe2+Cl4]2– [Fe2+EG3]4– [Fe3+Cl4]– [Fe3+EG3]3–

The reaction electronic energy (⊠E), Gibbs free energy (⊠G), enthalpy (⊠H), and HOMO-LUMO gap of these propose complexes computed with DFT can determine and predict which complex will most likely and most stably occur in the (1ChCl:2EG) DES medium. Results assist in understanding the iron speciation after being dissolved in (1ChCl:2EG) DES, and subsequently the electrochemical mechanism of pyrite dissolution in this system. The HPC-calculated DFT values can be confirmed experimentally by analysing the anodic dissolution of pyrite electrochemically, using AAS, ICP, UV-vis, or X-ray absorption fine structure (EXAFS). All calculations were performed using Gaussian 16, the B3LYP functional in gas phase and the PBEPBE Def2TZVP basis set. Each job typically ran for less than one hour on 24 processors and generates an output file of about 1 MB.

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Yes

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Session Classification: Micro-talks

Track Classification: Computational Chemistry