Quantum crystallographic quest for better ionic liquid based sorbents for N_2 and CO_2 removal from natural gas

This proposal seeks funding for an international IMPRESS-U collaboration involving University of Hawaii at Manoa and Warsaw University in Poland, aiming to engage colleagues and students from Ukrainian academic institutions in a project focused on development of selective sorbent materials for natural gas purification. Natural gas is one of the most valuable global fossil fuels resources and is a cornerstone of Ukraine's energy independence and security. This is particularly vital given the geopolitical conflict with Russia, as a robust domestic natural gas supply is essential for Ukraine's energy sovereignty. Beyond its strategic importance, natural gas is also a key economic driver, contributing significantly to the Ukrainian economy through job creation and revenue generation. From an environmental perspective, natural gas, being a cleaner-burning fossil fuel compared to coal and oil, offers Ukraine a path to reduce greenhouse gas emissions and mitigate air pollution.

Natural gas consists of a mixture of hydrocarbons with smaller amounts of carbon dioxide (CO_2), hydrogen sulfide, and nitrogen (N_2). Burning of natural gas contributes as much as 20% of total human-produced CO_2 emissions. CO_2 is highly corrosive, capable of damaging pipelines, and has very low energetic value. N_2, often found as an impurity in natural gas, or introduced during the fracking process, can lower the calorific value and efficiency of natural gas. CO_2 and N_2 removal leads to increased energy content per unit volume of gas, making it more efficient and economically viable. This not only has economic implications, reducing processing costs and enhancing the exploitation of natural gas fields, but also fosters technological advancements.

The current methods for removing CO_2 and N_2 from natural gas, such as physical and chemical absorption, water scrubbing, membrane separation, pressure swing adsorption, and cryogenic separation, face notable challenges. For instance, amine-based processes, while commonly used, struggle with issues like corrosion, amine degradation, solvent losses, and the need for energy-intensive regeneration. This is particularly problematic in the context of N_2 removal, where such drawbacks can significantly impact efficiency and cost-effectiveness. Moreover, physical absorbents, another common approach, have a high affinity to heavy hydrocarbons. This can lead to considerable hydrocarbon losses during the N_2 removal process, undermining the overall efficiency and economic viability of natural gas processing. As the global demand for natural gas surges, the urgency to develop more effective methods for N_2 removal becomes increasingly critical. In response to these challenges, ionic liquids are emerging as promising green solvents. Their nonflammability, negligible vapor pressure, and high chemical and thermal stability make them particularly appealing for N_2 and CO_2 removal applications. Preliminary studies have already demonstrated their potential in CO_2 removal from natural gas, but their effectiveness in N_2 removal remains a crucial area of research.

The selective absorption of gases like N_2 and CO_2 in porous sorbents is controlled by pore size and shape as well as charge distribution around sorption sites. **We will design, synthesize and characterize new improved selective sorbents based on solidified ionic liquids by integrating quantum crystallography and machine learning-driven structure search.** These ionic salts, composed of metal cations, imidazole-derivative cations, and dicarboxylic acid anion, are expected to offer a breakthrough in the efficiency and sustainability of N_2 removal. Quantum crystallography offers a new window into the microscopic world, allowing for an in-depth understanding of electronic structures and interactions between gas molecules and sorption sites and detailed map of charge distribution around the sorption sites. Machine learning-driven structure search utilizing structural and electron density features identified as key in controlling sorption allows to rapidly process vast libraries of potential compounds and quickly identify best candidates for efficient gas absorption. These algorithms not only facilitate the rapid screening of structures but also employ predictive modeling to forecast the performance of new sorbent structures. This predictive power is instrumental in speeding up the discovery process, allowing for the optimization and customization of sorbents for specific gases or environmental conditions. This integration is set to revolutionize the field, leading to the discovery of novel, more efficient solutions for the selective removal of N_2 and CO_2 from natural gas.