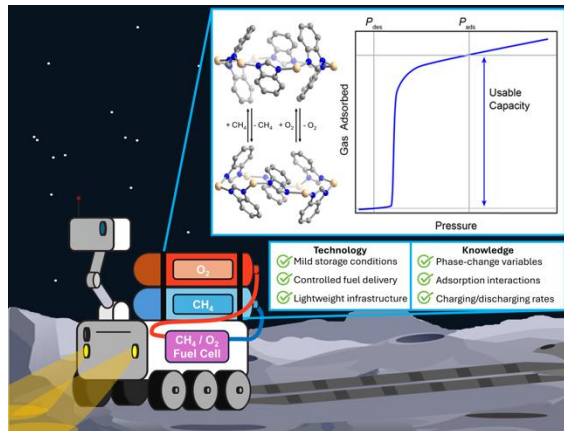


## Power on the Dark Side:

### Stimulus-Responsive Adsorbents for Low-Energy Controlled Storage and Delivery of Low Boiling Fuels to Mobile Assets in Permanently Shaded Regions

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We propose to study and develop stimulus-responsive cooperatively flexible adsorbents with step-shaped adsorption-desorption profiles capable of long duration storage, stable transport, and efficient delivery of  $\text{CH}_4$  and  $\text{O}_2$  under mild conditions in light tanks to power SOFCs in PSRs.

## Research Objectives

- We will study, develop, and deploy stimulus responsive adsorbents capable of storing, transporting, and delivering large capacities of  $\text{CH}_4$  and  $\text{O}_2$ , with lighter mechanical infrastructure and under milder physical conditions, to SOFCs for power generation in PSRs.
- Our work will enable: (i) breakthrough understanding of adsorption/desorption-induced phase changes in metal-organic frameworks, (ii) advanced knowledge of variables that influence  $\text{CH}_4$  and  $\text{O}_2$  noncovalent surface adsorption, (iii) unprecedented insights in the kinetics of desorption phase change adsorbents (iv) and more reliable and efficient power system technologies to be deployed with SOFCs in PSRs.
- SOA is storage of  $\text{CH}_4$  and  $\text{O}_2$  in liquid form, which requires extremely low temperatures and/or high pressures and heavy infrastructure that is prone to frequent off-gassing (i.e., fuel loss). Our efforts will enable the storage of large capacities of gaseous  $\text{CH}_4$  and  $\text{O}_2$  under more mild pressure/temperature conditions and controlled delivery with minor energy input. Enabling use of lighter tanks and reduced mechanical infrastructure on long duration missions.
- Start TRL = 1, End TRL = 3 or 4. The basic principle of step-shaped adsorption in flexible adsorbents has been shown. We will, at minimum, advance this to a critical function demonstration, ideally to a breadboard validation in the lab of high-capacity storage and regulated delivery of  $\text{CH}_4$  and  $\text{O}_2$ .

## Approach

- Our *hypothesis* is that by studying the fundamental variables regulating responsive phase changes and surface interactions for  $\text{CH}_4$  and  $\text{O}_2$  in cooperatively flexible metal-organic frameworks, we can intuitively modulate and/or design bespoke adsorbents for the storage and transport of  $\text{CH}_4$  and  $\text{O}_2$  in lightweight tanks and modular delivery of the gaseous fuels to SOFCs powering assets in Lunar and Martian PSRs.
- We pose three motivating questions and respective hypotheses, that when experimentally addressed will provide us with the knowledge to deliberately design and deploy adsorbents with the desired performance.
- Question 1: What variable(s) most strongly influence adsorbate-induced phase transitions for  $\text{O}_2$  and  $\text{CH}_4$ , respectively?
- Question 2: What variable(s) most strongly influence step shape—i.e., the slope or steepness—observed for adsorption and desorption under equilibrium conditions?
- Question 3: What variable(s) dictate if/how adsorption/desorption step shape is altered by changes in the rate of framework charging and discharging (i.e., storage and delivery)?
- These studies will be performed using chemical/materials synthesis, in situ X-ray diffraction, gas-phase adsorption-desorption experiments, NMR and FTIR spectroscopies, and DFT-level computations, amongst other techniques.

## Potential Impact

- The proposed work will accelerate the discovery and development of material adsorbent technologies that can help provide reliable power to future high-risk/high-payoff space science and exploration, specifically those leveraging SOFCs to power both mobile and long-duration assets in PSRs.
- This advancement will ultimately enable dramatic improvements at the system level, specifically in reducing the weight and cost of requisite infrastructure for compressing/cooling and storing low-boiling gaseous fuel, while also enhancing the reliability of storage and delivery of fuels to power non-solar illuminated small systems (Shortfall 1597) via SOFCs, as well as for long duration operations on the Moon and Mars (Shortfall 1595).
- The development of low-energy and controlled storage and delivery of gaseous fuels, such as  $\text{CH}_4$ ,  $\text{O}_2$ , and  $\text{H}_2$ , under mild pressure and temperatures can advance the viability of fuel cell technologies as alternative power sources on Earth.
- These investigations will also lead to fundamental knowledge of variables that influence the strength  $\text{CH}_4$  and  $\text{O}_2$  surface adsorption. These insights can be leveraged for the development of materials capable of capturing  $\text{CH}_4$  (a potent greenhouse gas) from point sources before emission into the atmosphere and for the low-energy purification of oxygen from air as an alternative to energy intensive cryogenic distillation currently deployed at massive industrial scales.