Bringing digital synthesis to Mars

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Using a fully automated closed-loop system, a robotic chemist synthesizes an oxygen-evolution catalyst from Martian meteorites, with implications for the production of catalysts that may underpin human survival on Mars in the future.

The discovery and development of new reactions, molecules and materials is highly complex and needs the integration of design, experiment and analysis for scientific understanding[1–5]. Recently, the digitization of chemistry[6] and materials discovery[7] has started to gain momentum, driven by the availability of fabrication methods and the development of machine learning methods[8]. These approaches are vital if we are going to use cutting-edge developments in data analysis and model building to accelerate science and to reduce the amount of labour involved in chemical discovery[9].

But beyond accelerating science in an Earthbound laboratory, what about doing science and materials discovery off-Earth? The idea of humanity becoming an interplanetary species, living freely among the stars, has long captivated science fiction enthusiasts. Yet today, extraterrestrial life, human or otherwise, remains confined to science fiction. The fact is that living in space is hard — very hard — and alien worlds present environments lethally hostile to terrestrial biology. If we wish to explore beyond the cradle of Earth to set up additional human civilizations in the Universe, then the utilization of local resources is essential: we must learn to live off the land. Settlers on Mars would need to obtain their own food, fuel and shelter rather than rely eternally on supply ships from Earth. Life-support essentials would have to be gleaned in situ, and that means that chemistry must be done on Mars.

Now, writing in *Nature Synthesis*, Shang, Jiang, Luo and co-workers provide an important step towards this goal[10]. Their artificial intelligence robotic chemist, the AI-Chemist, conceptually shows how it may be possible to help to unlock the potential of the red planet, providing a beachhead on which to build the infrastructure needed to support life. By demonstrating automated synthesis of an oxygen-evolving electrocatalyst using meteorites from Mars as the raw material, they prove the concept of developing vital materials and infrastructure for Martian exploration through automated in situ resource utilization (ISRU). Their robotic platform integrates materials analysis, computational molecular design and autonomous synthesis in a closed-loop system that needs only a power supply and raw feedstock ores to produce oxygen. The AI-Chemist showcases the disruptive potential of AI and robotics when combined with the dizzying complexity of chemistry and materials science on another planet.

While inspirational as a proof-of-concept, the current robotic system relies on fixed equipment rather than roving autonomous platforms (Fig. 1). It has been tested only under simulated Martian conditions within the controlled confines of an Earthbound laboratory.
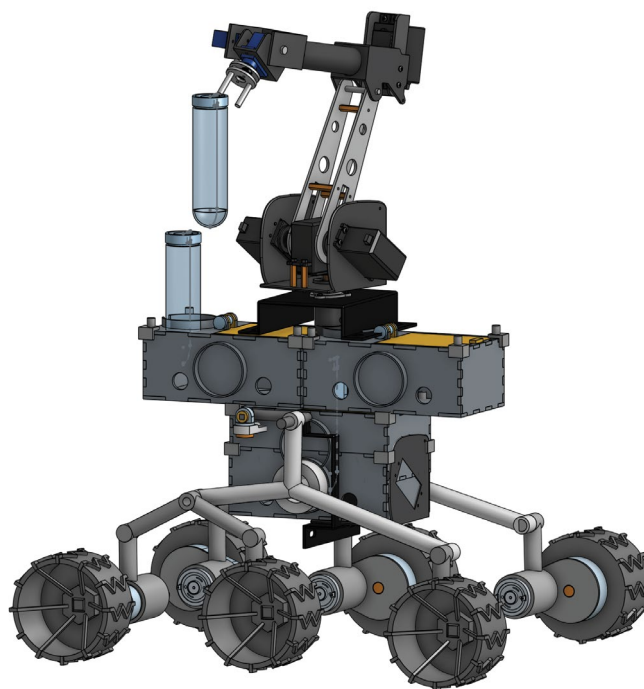

Fig. 1 | A putative autonomous materials chemistry robot rover.

The harsh radiation, dust storms and temperature extremes of Mars remain beyond its operational limits. The catalyst itself, although produced from materials likely to be present on Mars, performs much worse than state-of-the-art commercial oxygen-evolution electrocatalysts. The effect of Mars' reduced gravity relative to Earth on the electrolysis process (or on the robotic system itself) could be substantial[11] and remains unexplored. Truly living off Mars would require mobility and resilience, and the ability to interact directly with the landscape, beyond the safety of a controlled habitat. Reactive chemistry and complex manufacturing are difficult enough on Earth; conducting them reliably on another planet will require rugged, adaptive systems and will stretch the limits of autonomy.

However, such criticisms miss the crucial point of the work by Shang, Jiang, Luo and colleagues[10]. The conditions may be somewhat contrived, and the catalysts that were obtained may not be best-in-class, but the methods by which the catalysts were produced, tested and optimized are general, as well as being applicable (and useful) for ISRU. Producing oxygen extraterrestrially from local resources will surely be one of the main enabling processes for independent off-Earth habitation. The Mars Oxygen ISRU Experiment (MOXIE) has demonstrated successful oxygen production from the Martian atmosphere[12], but it uses a platform constructed entirely on Earth. Other approaches for

in situ generation of oxygen from local off-Earth resources may allow direct production of oxygen from planetary regolith itself[13] but are not yet fully developed.

The prospect of deploying machine learning and AI to develop and optimize both the hardware and chemistry underlying ISRU processes is highly attractive: it may transform our ability to live on other worlds. Mars and the Moon are obvious destinations, but other more audacious targets include Saturn's moon Titan (which has abundant ice and evidence of an atmosphere containing organic chemicals: ideal building blocks of feedstocks for fuels, plastics and fertilizers), and the Solar System asteroids rich in ice and (potentially precious) minerals. The sheer diversity of extraterrestrial targets suggests that producing individual ISRU systems on Earth for each instance will be time-consuming, costly and inefficient. Harnessing machine learning and AI could allow adaptive and adaptable resource-harvesting robotic scouts to adjust to almost any environment autonomously.

To transform this science fiction into reality, our robotic chemists must be mobile, durable and intelligent enough to live off the land, whether that be the sands of Mars or the icy realm of Titan. By integrating automation, autonomy and molecular processes they may yet build oases wherever humans wish to roam.

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