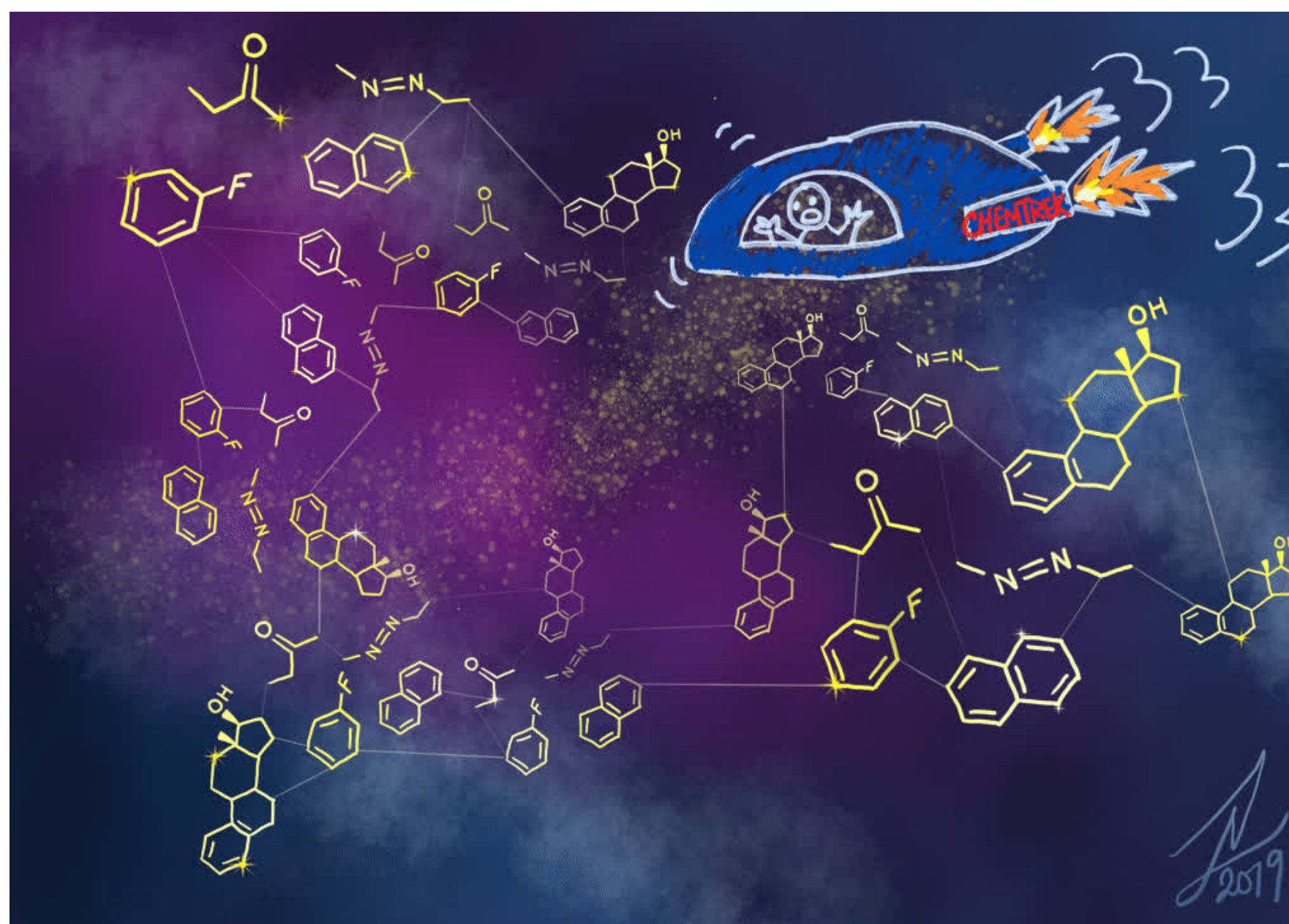




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Is Chemical Space Designed or Discovered?



What defines chemical space and how can it be searched or designed from the bottom up? How can discovery be 'focused' into a desired property search for the design of novel materials with advanced properties? Is it possible to design the discovery of materials using theory and experiment joined together with autonomous systems? More speculatively what are the limits on life elsewhere in the universe and chemical space?

In my lecture I will address these three important questions demonstrating how we have developed new approaches to explore chemical space using probabilistic approaches, design of experiments and machine learning to enable the mapping and discovery of new molecules, materials, formulations, and nanostructures. To do this we have built closed-loop platforms that incorporate the design of new properties, quantum theory, machine learning, modular chemical reactions, and testing of the products all in real time using an autonomous modular robotic system we call the Chemputer. Because the Chemputer is the worlds first and only modular and universal programmable materials synthesis and discovery robot, we can develop highly efficient and novel routes to explore the space of new matter according to radical new design strategies, desired physical properties, and looking also for the discovery of new physical phenomena and to brute force the origin of life.

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