**////Title: Exploring the Surface Chemistry of Interstellar Dust**

**////Standfirst:**

Interstellar space may seem like the last place you would look when searching for the chemical origins of life. Yet on the surfaces of tiny dust grains within this vast expanse, complex chemical reactions are continually occurring, which likely played a key role in establishing the rich diversity of complex molecules we observe in the solar system today. In a new study, astrochemists in Spain and Italy, led by Albert Rimola at the Autonomous University of Barcelona, examine how advanced simulation techniques can be used to study these important processes on atomic scales.

**////Main text:**

When we envisage the origins of the complex chemicals that form the building blocks of life, we often think about dynamic environments such as oceans, atmospheres, and planetary interiors. However, the rich array of molecules we observe today didn’t entirely originate within our solar system.

Instead, many molecules are synthesised on the surfaces of carbon- or silicon-based dust grains less than one micrometre in size, which float through interstellar space. These materials are often coated with a layer of ‘dirty’ ice containing an abundance of organic molecules. Furthermore, the unique structures of their surfaces are believed to act as binding or catalytic sites – allowing complex chemical reactions to occur.

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The story of this process begins when an old, dying star ejects its gas and dust – forming an interstellar cloud which cools and contracts over time. Hydrogen molecules are abundant at this stage, and react with oxygen and carbon on dust grain surfaces to form simple molecules such as methanol and water – coating dust grains with dirty icy layers.

As the cloud continues to collapse under its own gravity, its dense core may heat up, and begin to form a new star. This heating releases the frozen molecules on any nearby dust grains, triggering the formation of organic molecules including alcohols, ethers, and aldehydes. From here, the remaining gas and dust collects into a disk encircling the star – which over time, will coalesce to form asteroids, comets, and even planets.

In the coldest regions of these ‘protoplanetary’ disks, these more complex molecules become re-frozen on grain surfaces. This introduces further chemical complexity – potentially producing biological molecules such as amino acids, sugars, and nucleobases. However, researchers still know very little about how this chemistry unfolds.

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So far, our knowledge of these processes has been shaped by a combination of strategies – including theoretical models, lab experiments, and astronomical observations – where the fingerprints of certain chemicals are contained in the infrared radiation emitted by dust grains. So far, these techniques have allowed astrochemists to identify and qualify chemical species in a variety of interstellar environments, providing key clues as to how the molecular diversity of our solar system first emerged.

However, each of these approaches comes with its own shortcomings, which prevent them from providing an atomic-scale picture of how important chemical processes occur. So far, this has prevented astrochemists from gaining a full understanding of how complex molecules form in interstellar space, calling for a new generation of more advanced techniques.

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To overcome these limitations, Dr Albert Rimola at the Autonomous University of Barcelona turns to computational chemistry. This interdisciplinary approach uses computer simulations to represent the elementary steps of complex chemical reactions on a molecular scale. Such steps include the binding of molecules onto dust grains, reactions with other molecules, and the eventual release of the resulting chemical products from the dust grains.

Computational chemistry has been widely used to explore the chemistry of surfaces such as metals and metal oxides, but so far, their use in the specific field of astrochemistry has been far less extensive. In a recent study, Dr Rimola and his colleagues explored a variety of approaches that can be used to mimic the surfaces of interstellar dust grains, and simulate the chemical processes they enable in a realistic way. Their paper presents all of the state-of-the-art methods, techniques, and strategies currently available, and examines their unique advantages and shortcomings.

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The first approach explored by the team are ‘quantum chemical’ methods, which use calculations based on quantum mechanics to determine how individual electrons and atomic nuclei interact with each other. This can be done in a number of possible ways, which use different mathematical descriptions of electron distributions within atoms. Quantum chemistry allows for incredibly precise simulations – but due to its immense complexity, these models are limited to sizes of just hundreds of atoms.

Alternatively, this approach can be combined with lab experiments and astronomical observations. This is far quicker and less costly, allowing researchers to simulate larger chemical systems – but comes with the risk of far lower accuracy, if the simulated system’s parameters aren’t carefully chosen.

The second approach describes classical molecular dynamics simulations. These ignore electrons and their motions, and instead describe chemical systems using ‘ball and spring’ models – where atoms are the ‘balls’ of differing sizes and softness; and their bonds are ‘springs’ of varying stiffness. This approach is less accurate, but its reduced complexity allows researchers to simulate systems containing thousands of atoms. This enables them to recreate complex molecular systems without the risk of incurring significant errors, but not chemical processes involving electron reorganisation, such as chemical reactions.

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By drawing these differing approaches together, and assessing their capabilities in detail, Dr Rimola and his colleagues hope that their study could spark a wave of research into the computational chemistry of interstellar dust grains. The scope of their research may also expand to consider the surface chemistry of comets and asteroids – which may have delivered many of the molecular building blocks of life to Earth’s surface.

As a result, the team believes that the latest advances in computational chemistry could soon offer new clues about the emergence of life on Earth, and potentially even planets beyond our solar system.

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This SciPod is a summary of the paper ‘Computational Surface Modelling of Ices and Minerals of Interstellar Interest—Insights and Perspectives’, from Minerals. [doi.org/10.3390/min11010026](https://www.mdpi.com/2075-163X/11/1/26)

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