Hop, skip and a jump: Researchers reveal molecular search patterns

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Like an albatross scanning for pods of squid in a vast ocean, molecules on solid surfaces move in an intermittent search pattern that provides maximum efficiency, according to new research from the University of Colorado Boulder.

While this behavior had been proposed theoretically, CU-Boulder researchers have made the first experimental observations of this phenomenon, providing a gateway for potential improvements in fields ranging from medical diagnostics to chemical production.

"Cutting-edge technologies like lab-on-a-chip devices and biosensors rely on molecules quickly and effectively interacting with the targets they're seeking," said Professor Daniel Schwartz of the Department of Chemical and Biological Engineering. "By better understanding exactly what's happening at the molecular level, we can enhance or engineer technologies that operate faster and more efficiently. Possible outcomes might include a more robust response to disease markers, a less wasteful technique for commercial chemical production or any number of other advances."

The research, conducted by Schwartz and Jon Monserud, a PhD candidate in the Department of Chemical and Biological Engineering, was recently published in the journal *Physical Review Letters*.

In nature and society, everything from predatory animals to submarine-seeking ships has developed search strategies where slow, localized searches alternate with long, non-searching movements to explore vast areas where targets are sparse, Schwartz said. When prey is abundant, a simple random walking method is a better way to make connections.

Researchers wondered if molecules would behave the same way.

To examine the theory, researchers used single-molecule tracking to directly observe the search process of DNA on surfaces decorated with complementary DNA and witnessed periods of slow motion punctuated by fast hops through an adjacent liquid phase.

By measuring how long it took for each molecule to find its target, researchers determined that the tiny particles were indeed using the same intermittent-flight foraging techniques as a shark hunting for prey or a honeybee seeking nectar. This strategy allowed them to find targets more than 10 times faster than they would have using a simple random walk search.

"It's an incredible coincidence that molecules are exhibiting the same counterintuitive methods that animals and humans have evolved or chosen to use," said Monserud. "We can exploit this coincidence to improve a wide range of technologies."

In the medical field, for example, detection tests for scores of diseases rely on biomarkers such as antibodies or mutated DNA reacting to probe molecules on surfaces to inform doctors of the presence or severity of a malady.

The researchers demonstrated that molecules searched more quickly on hydrophobic surfaces, indicating that developers of DNA biosensors could benefit from tailoring their diagnostic products to have more wateraverse surfaces. The findings may result in quicker diagnoses, individually tailored healthcare, and potentially, better outcomes for patients.

The findings could also optimize industrial production to reduce energy, time, materials and costs. In many industrial processes, raw materials are converted to fuels, pharmaceuticals or personal care products through chemical reactions, then separated from the remaining waste. Both the reactions and purification processes require molecules to scan surfaces and bind to targets through the same intermittent searching behavior.

"In a sense, our findings help explain why these technologies surprisingly work as well as they do," Schwartz said. "But additionally, developing this understanding can potentially help us design even better technologies since, until now, people have always assumed that molecules searched in a different manner."

More information: Jon H. Monserud et al. Interfacial Molecular Searching Using Forager Dynamics, *Physical Review Letters* (2016). DOI: 10.1103/PhysRevLett.116.098303

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