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Nano propellers pump with proper chemistry

The ability to pump liquids at the cellular scale opens up exciting possibilities, such as precisely targeting medicines and regulating flow into and out of cells. But designing this molecular machinery has proven difficult.

Now chemists at the University of Illinois at Chicago have created a theoretical blueprint for assembling a nanoscale propeller with molecule-sized blades.

The work is featured in Research Highlights in the July 12 issue of Nature and was described in the June 28 cover story of Physical Review Letters.

Using classical molecular dynamics simulations, Petr Král, assistant professor of chemistry at UIC, and his laboratory coworkers were able to study realistic conditions in this microscopic environment to learn how the tiny propellers pump liquids.

While previous research has looked at how molecular devices rotate in flowing gases, Král and his group are the first to look at molecular propeller pumping of liquids, notably water and oils.

“We want to see what happens when the propellers get to the scale where it’s impossible to reduce the size of the blades any more,” said Král.

Král’s group found that at the molecular level — unlike at the macro level — the chemistry of the propeller’s blades and their sensitivity to water play a big role in determining whether the propeller pumps efficiently or just spins with little effect. If the blades have a hydrophobic, or water-repelling nature, they pump a lot of water. But if they are hydrophilic — water-attracting — they become clogged with water molecules and pump poorly.

“Pumping rates and efficiencies in the hydrophilic and hydrophobic forms can differ by an order of magnitude, which was not expected,” he said.

The UIC researchers found that propeller pumping efficiency in liquids is highly sensitive to the size, shape, chemical or biological composition of the blades.

“In principle, we could even attach some biological molecules to the blades and form a propeller that would work only if other molecules bio-compatible with the blades are in the pumped solution,” he said.

The findings present new factors to consider in developing nanoscale liquid-pumping machines, but Král added that such technology probably won’t become reality for several years, given the difficult nature of constructing such ultra-small devices.

Král’s laboratory studies how biological systems, like tiny flagella that move bacteria, offer clues for building motors, motile systems and other nanoscale devices in a hybrid environment that combines biological and inorganic chemistry.

“The 21st century will be about hybrid biological and artificial nanoscale systems and their mutual co-evolution,” Král predicts. “My group alone is working on about a half-dozen such projects. I’m optimistic about such nanoscale developments.”

Source: University of Illinois at Chicago

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