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.

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....

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