

What a ride! Researchers take molecules for a spin (w/ Video)

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(PhysOrg.com) -- Kolomeisky and Rice graduate student Alexey Akimov have taken a large step toward defining the behavior of these molecular whirligigs with a new paper in the American Chemical Society's Journal of Physical Chemistry C. Through molecular dynamics simulations, they defined the ground rules for the rotor motion of molecules attached to a gold surface.

"This is no cartoon. It's a real molecule, with all the interactions taking place correctly," said Anatoly Kolomeisky as he showed an animation of atoms twisting and turning about a central hub like a carnival ride gone mad.

Kolomeisky, a Rice University associate professor of chemistry, was offering a peek into a molecular midway where atoms dip, dive and soar according to a set of rules he is determined to decode.

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It's an extension of their work on Rice's [famed nanocars](#), developed primarily in the lab of James Tour, Rice's T.T. and W.F. Chao Chair in Chemistry as well as a professor of mechanical engineering and

materials science and of computer science, but for which Kolomeisky has also constructed molecular models.

Striking out in a different direction, the team has decoded several key characteristics of these tiny rotors, which could harbor clues to the ways in which molecular motors in human bodies work.

The motion they described is found everywhere in nature, Kolomeisky said. The most visible example is in the flagella of bacteria, which use a simple rotor motion to move. "When the flagella turn clockwise, the bacteria move forward. When they turn counterclockwise, they tumble." On an even smaller level, ATP-synthase, which is an enzyme important to the transfer of energy in the cells of all living things, exhibits similar rotor behavior -- a Nobel Prize-winning discovery.

Understanding how to build and control molecular rotors, especially in multiples, could lead to some interesting new materials in the continuing development of machines able to work at the nanoscale, he said. Kolomeisky foresees, for instance, radio filters that would let only a very finely tuned signal pass, depending on the nanorotors' frequency.

"It would be an extremely important, though expensive, material to make," he said. "But if I can create hundreds of rotors that move simultaneously under my control, I will be very happy."

The professor and his student cut the number of parameters in their computer simulation to a subset of those that most interested them, Kolomeisky said. The basic-model molecule had a sulfur atom in the middle, tightly bound to a pair of alkyl chains, like wings, that were able to spin freely when heated. The sulfur anchored the molecule to the gold surface.

While working on a previous paper with researchers at Tufts University,

Kolomeisky and Akimov saw photographic evidence of rotor motion by scanning tunneling microscope images of sulfur/alkyl molecules heated on a gold surface. As the heat rose, the image went from linear to rectangular to hexagonal, indicating motion. What the pictures didn't indicate was why.

That's where computer modeling was invaluable, both on the Kolomeisky lab's own systems and through Rice's SUG@R platform, a shared supercomputer cluster. By testing various theoretical configurations -- some with two symmetrical chains, some asymmetrical, some with only one chain -- they were able to determine a set of interlocking characteristics that control the behavior of single-molecule rotors.

First, he said, the symmetry and structure of the gold surface material (of which several types were tested) has a lot of influence on a rotor's ability to overcome the energy barrier that keeps it from spinning all the time. When both arms are close to surface molecules (which repel), the barrier is large. But if one arm is over a space -- or hollow -- between gold atoms, the barrier is significantly smaller.

Second, symmetric rotors spin faster than asymmetric ones. The longer chain in an asymmetric pair takes more energy to get moving, and this causes an imbalance. In symmetric rotors, the chains, like rigid wings, compensate for each other as one wing dips into a hollow while the other rises over a surface molecule.

Third, Kolomeisky said, the nature of the chemical bond between the anchor and the chains determines the rotor's freedom to spin.

Finally, the chemical nature of rotating groups is also an important factor.

Kolomeisky said the research opens a path for simulating more complex rotor molecules. The chains in ATP-synthase are far too large for a simulation to wrangle, "but as computers get more powerful and our methods improve, we may someday be able to analyze such long [molecules](#)," he said.

More information: Dynamics of Single-Molecule Rotations on Surfaces that Depend on Symmetry, Interactions, and Molecular Sizes, J. Phys. Chem. C, 2011, 115 (1), pp 125–131. [DOI: 10.1021/jp108062p](https://doi.org/10.1021/jp108062p)

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