24 Hours of Toulouse

On a Thursday in March 2022, scientists from three continents gathered in Toulouse, France, to crown the best among eight international molecular racing teams competing in the second edition of the NanoCar Race.

nce a year, motorsport enthusiasts from all around the globe meet in the northwest of France, halfway between Paris and Nantes, to celebrate the 24 Hours of Le Mans, an endurance sports car race with a history in long distance racing of almost one century. 500 km further south, in Toulouse, on 24 March this year, another endurance race took place for the second time, the NanoCar Race (https://www.memo-project.eu/ flatCMS/index.php/Nanocar-Race-II). Eight interdisciplinary teams from three continents came together to see who could drive a single molecule over the largest distance within 24 hours.

Instead of gasoline, electrical pulses from the tip of a scanning tunnelling microscope (STM) propel the cars, which consist of only about 100 atoms and are 9 orders of magnitude smaller than their Le Mans cousins. Instead of 5,000 km on a tarmac circuit, the molecular cars move along a slalom path, defined by the naturally occurring herringbone reconstruction on the (111) cut of a gold single crystal. Following tracks of different difficulty, the two winning teams covered 680 nm and 1,050 nm, respectively.

But how are such small cars steered? Christian Joachim, the organizer of the event and CEMES-CNRS researcher, explains that two types of 'engines' may propel the nanocars: in the first, dipolar engine, a pulsed electric field, generated at the apex of the STM tip attracts the molecule and moves it along the surface; in the second, inelastic engine, tunnelling electrons inelastically provide energy to vibrations of the molecule, moving the 'car' over the diffusion barrier on the gold surface. Both engines require an exact positioning of the tip, with a precision well below the diameter of an atom. According to Joachim, a combination of the two types of propulsion, similar to a hybrid car that uses both a combustion and an electrical engine, probably works best. He is impressed by how nicely the molecular cars executed "such a complex task: go straight, turn left, turn right and sidestep obstacles".



The NanoCar Race II took place in the Boule in Toulouse, home to the 1.3 MeV accelerator of a retired electron microscope. Credit: CEMES-CNRS F. Maligne

To achieve such a high degree of control, the two winning teams decided on rather antithetical design principles. The NANOHISPA team from IMDEA Nanociencia in Madrid, Spain, which was led by David Écija, Emilio Pérez, and Koen Lauwaet, synthesized a rather small molecule with a form reminiscent of an actual car. 70 atoms were enough to form an anthracene chassis and toluene rear wheels and benzene front wheels. The small size and the addition of wheels, which reduce the interaction of the chassis with the gold surface, enables easy motion along the tracks.

Instead of reducing interaction, the NIMS-MANA team from Tsukuba, Japan, went for a minimal friction strategy. Shigeki Kawai, the driver of the team, explains that they employed the concept of superlubricity, a regime where the friction between two touching surfaces reduces dramatically or even vanishes completely. Back in 2016, Kawai together with colleagues from Switzerland, Germany and Spain, discovered that graphene nanoribbons could move over a gold surface in a superlubric state¹. For NanoCar Race II, they designed a large and flat molecule with a chemical structure reminiscent of graphene nanoribbons and forwent wheels completely. Their car adsorbs strongly onto the surface,

but may have a very small diffusion barrier thanks to superlubricity.

Another tweak to the concept was that the NIMS-MANA team, which was led by Tomonobu Nakayama, assembled the car directly on the race track. They employed on-surface synthesis to produce the final, complex molecule from smaller, simpler, and more stable precursor molecules, which can be easily deposited on the gold surface without damage. While this approach surely comes with some downsides, by doing so, they prevented decomposition of the nanocar during the deposition procedure, which usually involves high temperatures or high kinetic energy.

In the surface science community, on-surface synthesis has become fashionable in the last decade², as it allows constructing large molecular structures in a clean environment. These molecules would be otherwise hard to deposit on a surface without damage or, in some cases, even impossible to synthesize without the two-dimensional confinement provided by the surface as in the case of triangulene³.

When asked what they have learned from the competition, Écija, technical team lead of the NANOHISPA team, mentioned the insights gained into the efficient manipulation of molecules on surfaces and how this will be valuable in daily lab routines in future. Then he emphasized the importance of outreach for modern science and finished saying: "It was fantastic to transmit our passion for nano to a broad audience, including our relatives and friends." We have nothing to add! If you missed the live broadcast, you can watch the full 24 Hours of Toulouse, here at https://www.youtube.com/ watch?v=JRmA7jI_usg.

Published online: 17 May 2022 https://doi.org/10.1038/s41565-022-01143-y

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