Solving single molecule mobility

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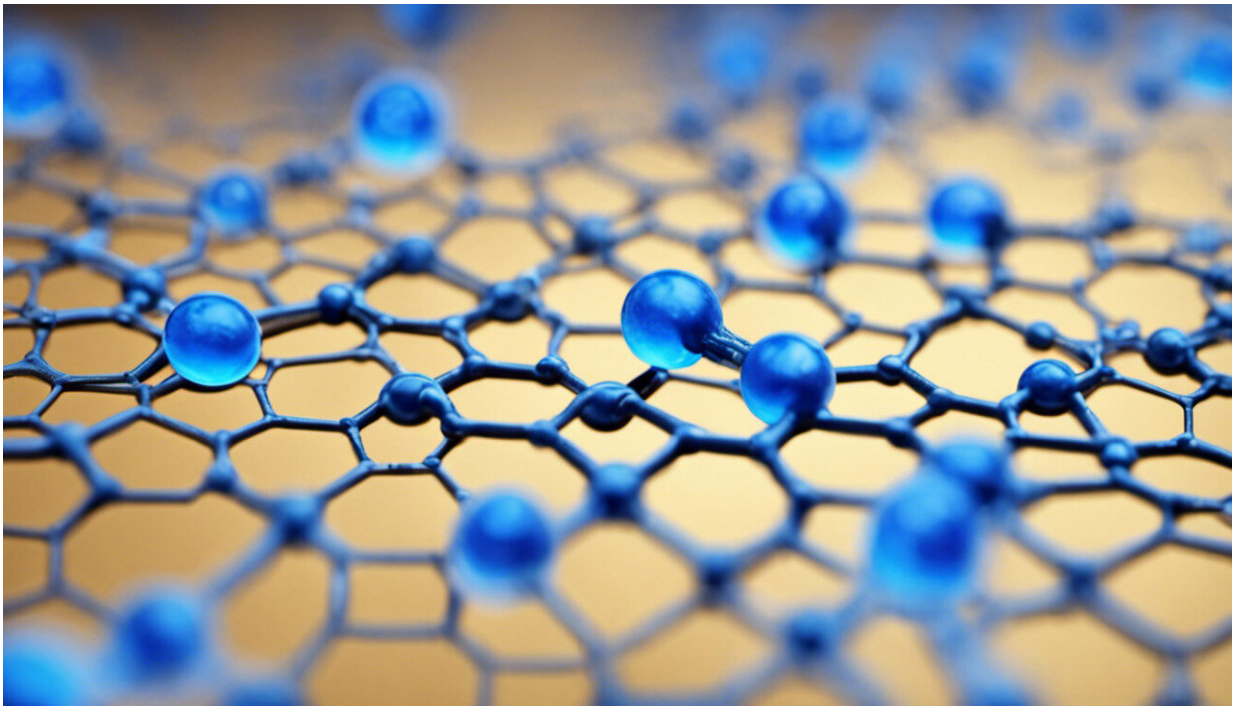

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Nanotechnologists assemble intricate nanodevices, such as computer chips, molecule by molecule using 'bottom-up' techniques that mirror nature. One approach shuttles molecules along surfaces into new and functional arrangements using electrons from a scanning tunneling microscope (STM) tip. However, because energy transfer between the atomic-scale tip and the surface chemical involves many complex interactions, laborious efforts are currently needed to understand even

the simplest reactions.

Results from a new theoretical and experimental study, however, may soon allow non-specialists to easily construct molecular devices. Kenta Motobayashi and Yousoo Kim from the RIKEN Advanced Science Institute in Wako and their colleagues from RIKEN and Japanese universities have developed a mathematical formula that describes how STM-induced molecular vibrations couple with dynamic movements on surfaces—enabling precise calculation of the energy and number of electrons needed to initiate single molecule motions.

When scientists use an STM to perform a straightforward molecular movement—for example, making carbon monoxide (CO) compounds 'hop' on palladium surfaces—they see that the fraction of successful movements depends heavily on the applied voltage. For CO, this is because hopping from one surface site to another requires a tunneling electron to initiate a specific stretching vibration. In the voltage range corresponding to this vibrational energy, CO hopping can increase exponentially, giving rise to so-called 'action spectra': curves of movement yields versus voltage with shapes characteristic to particular surface reactions.

Motobayashi, Kim and colleagues sought to uncover the microscopic mechanisms behind STM-stimulated diffusion by proposing a formula that relates movement yields to the energy transfer efficiency needed to excite reaction-triggering vibrations, while also accounting for thermal interactions. Fitting the CO action spectra to this formula revealed the exact magnitudes of critical reaction properties, like vibrational energies and rate constants, because the spectral curves were highly sensitive to small modification of the fit parameters.

Furthermore, the team's new equation proved versatile enough to analyze the more complex motions of butene (C_4H_8) molecules on palladium, a

process that involves multiple excitations. Analyzing the butene action spectra with the formula showed the presence of three distinct vibrations and enabled calculation of the reaction order—a fundamental chemical property that identifies the number of tunneling electrons needed to initiate surface movement.

According to Motobayashi, the surprising abilities of this simple method should expand bottom-up nanotechnology practices. “STM-based action spectroscopy, which can precisely identify chemical species thanks to our spectral fittings, promises to contribute greatly to the technique of composing molecular devices,” he states.

More information: Motobayashi, K., et al. Insight into action spectroscopy for single molecule motion and reactions through inelastic electron tunneling. *Physical Review Letters* 105, 076101 (2010). prl.aps.org/abstract/PRL/v105/i7/e076101

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