



# Molecular Disjunctions: Staking Claims at the Nanoscale

Alfred Nordmann

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## ABSTRACT

Nanoscience may be surrounded by controversy but is characterized by its absence. Evidence for this comes from the reconstruction of a peculiarly muted scientific "debate" regarding the claim that a single organic molecule may serve as a wire in electronic circuitry. Even though there are fundamentally different theoretical approaches, the debate remains entirely implicit. This is because the research in question is motivated by interest neither in a true representation of nature, nor simply in the invention of devices or production of new substances. As a place-oriented enterprise NanoTechnoScience consists mostly in the settlement and staking of claims on the nanoscale.

## I. NANOTECHNOSCIENCE

The main thesis of this paper was motivated and explicated elsewhere (Nordmann 2002, 2004a, 2004b). What follows is an attempt to substantiate it with the help of a particular case study. To be sure, this is nothing like testing a hypothesis; at best, it will render the thesis more plausible and concrete.

Nanoscience is not an issue-driven but a place-oriented enterprise. It is neither interested in representations of nature nor in devices that work or substances with novel properties. Truth/falsity and confirmation/refutation do not serve as its epistemic standards, but epistemic success is also not measured in terms of functionality of devices or usefulness of substances. Instead, nanoscience is an exploratory attempt to claim foreign territory and to inhabit a new world or an hitherto unexplored region of the world. Epistemic success is therefore a kind of technical achievement, namely the ability to act on the nanoscale, that is, to see, to move around, move things around, carve your name into a molecule, perhaps initiate productive processes, in other words, to inhabit inner space somewhat as we have begun to inhabit outer space and certainly as we have conquered the wilderness.<sup>1</sup>

This passage speaks of nanoscience as opposed to nanotechnology. Roughly speaking, nanoscale research concerns molecular architecture, nanotechnology aims for the control of this architecture, and nanoscience investigates the physical properties that depend on it.<sup>2</sup> However, if the thesis is correct, it turns out that even nanoscience isn't "science" properly or traditionally speaking, and that even for nanoscience there is no distinction between theoretical representation and technical intervention, between understanding nature and transforming it. More properly one should therefore speak of NanoTechnoScience.<sup>3</sup>

First, some *prima facie* evidence will be presented for the thesis. It comes from the general area of molecular electronics. The initial impressions obtained from this will then be traced to two culturally distinct research groups that appear to be working on the same problem. Trying to identify in their writings the core commitments of both groups, one finds that one of them seeks to identify and solve "fundamental problems" and that this orientation marks a rather fundamental disagreement between the two research groups. However, this disagreement remains entirely implicit and does not become subject of debate. Like the lack of scientific discussion on such basic issues as the physical possibility of "molecular assemblers," this lack of debate can be taken as evidence for the thesis of a non-traditional NanoTechnoScience that is not driven by theoretical issues but consists mostly in the settlement and staking of claims on the nanoscale.<sup>4</sup> Nanoscience may be surrounded by controversy but here it proves to be characterized by its absence.

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1. The metaphor of inner and outer space was introduced by Sean Howard (2002) in the context of his discussion of military applications of nanotechnology and the need for an "inner space treaty."

2. This definition was adapted from a presentation by Cathy Murphy at the "Reading Nanoscience" workshop, University of South Carolina, August 2002.

3. An "issue-driven" scientific research programme is oriented towards "problems" in the sense discussed by Kuhn (where a paradigm defines the problems of research and where science progresses by solving the outstanding problems or puzzles). It might also be oriented towards a problem like the cure of cancer or the creation of artificial intelligence. As a whole, neither of this holds for Nanoscience. Instead, the "place-orientation" refers to the claiming and inhabiting of a space. Learning to move around, to act and be productive in this space is no easy task but does not involve "problems" in the previously mentioned senses.

4. The recent exchange of letters between Richard Smalley and Eric Drexler serves only to highlight this absence of a sustained scientific debate (Baum 2003).

## II. PRESSING PROBLEMS

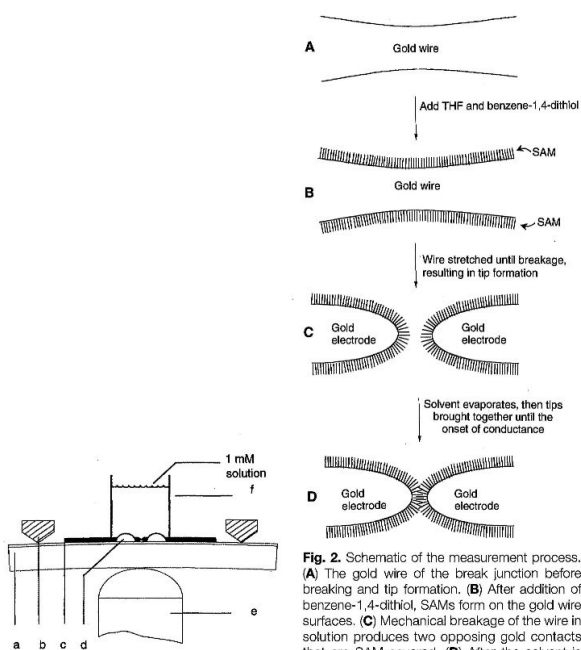
In a September 2002 presentation Stan Williams identified a problem that "must be solved": How are electrons going through molecules? This is a question for molecular electronics. It is accompanied by another question: Why is this such a pressing problem, what makes it so interesting?

There are two kinds of answers to this latter question. One of these belongs to an issue-driven enterprise, the other characterizes the place-orientation of NanoTechnoScience. According to the thesis, one wouldn't expect the first of these or one like it offered at all. As we will see, it may not be quite that simple.

This first kind of answer requires for a foil the history of physics at least since the time of Faraday and Maxwell. As Jed Buchwald, in particular, has pointed out, they effected a transformation of physical thinking that prepared the ground also for quantum mechanics (Buchwald 1985). Physical effects were not to be attributed to spatio-temporally localized causes but to space itself which is no longer a mere medium for the transmission of effects as they traverse from their point of origin to a detector, but, in a sense, the space itself can get excited and the change of its state communicated. The propagation of effects therefore does not require particles on which they ride or by which they are transported – all this most famously exemplified in electrodynamics by the propagation of radio waves.

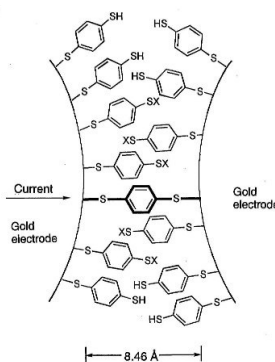
Against this background, the question of how electrons travel through molecules takes on a particular significance. In physical, though not perhaps in chemical terms, it presupposes a curiously old fashioned picture, one according to which a molecule is a discrete kind of body which first is penetrated by and from which then exits another body, namely an electron. Since this electron carries a charge, the passage of the electron through the molecule is associated with a flow of a current and the question by Stan Williams amounts to: Is a molecule qua molecule something like a channel through which current is propagated differently than it is through space on the one hand, through bulk material on the other? If yes, the shape and structure of molecules is physically significant (Woolley 1978). Furthermore, if molecules are conductors of electricity and, so to speak, channel the flow of electrons, do the same laws apply to them as to bulk material? In particular, do they offer a resistance to this flow that serves as a constraint on the amount of current such that too high a voltage would generate so much heat that the molecule ought to melt like a wire that is too thin (compare Di Ventra et al. 2002, 195)?

All this is terribly crude and simple-minded. It certainly does not even begin to reflect the availability of theoretical models that propose answers to Stan Williams's question. But then Williams was not asking for a theoretical model but for an empirical determination. How do electrons move through molecules? Experimental answers to this question can be traced to Mark Reed and Jim Tour's 1997 paper in *Science* on the "Conductance of a Molecular Junction" (Reed et al. 1997). Reed and Tour provide experimental evidence combined with statistical argumentation to distinguish current flow through a single organic molecule from the current that may or may not be propagated in its immediate environment. They use bulk material to create a so-called break junction where two coated gold electrodes are slowly moved together until conductance is achieved (Figure 1). Presumably, this happens exactly when atoms in the coating self-assemble into a first molecular bridge between the parabolically shaped electrodes. Figure 3 illustrates just how precarious a process this is: There is a lot going on in the space between the electrodes, and the experiment is to determine that the measured current is flowing through the single molecule and nowhere else. A first indication of the experiment's success was the fact that the distance of the electrodes when conductance is achieved agreed fairly closely with the calculated length of the single molecule that formed the bridge, namely roughly 8 angstrom.

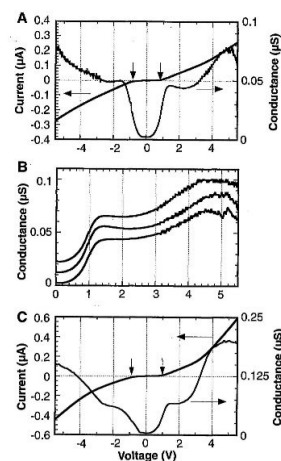


**Fig. 2.** Schematic of the measurement process. (A) The gold wire of the break junction before breaking and tip formation. (B) After addition of benzene-1,4-dithiol, SAMs form on the gold wire surfaces. (C) Mechanical breakage of the wire in solution produces two opposing gold contacts that are SAM-covered. (D) After the solvent is evaporated, the gold contacts are slowly moved together until the onset of conductance is achieved. Steps (C) and (D) (without solution) can be repeated numerous times to test for reproducibility.

**Fig. 1.** A schematic of the MCB junction with (a) the bending beam, (b) the counter supports, (c) the notched gold wire, (d) the glue contacts, (e) the piezo element, and (f) the glass tube containing the solution.



**Fig. 3.** A schematic of a benzene-1,4-dithiolate SAM between proximal gold electrodes formed in an MCB. The thiolate is normally H-terminated after deposition; end groups denoted as X can be either H or Au, with the Au potentially arising from a previous contact/retraction event. These molecules remain nearly perpendicular to the Au surface, making other molecular orientations unlikely (27).



**Fig. 4.** (A) Typical  $I(V)$  characteristics, which illustrate a gap of 0.7 V; and the first derivative  $G(V)$ , which shows a step-like structure. (B) Three independent  $G(V)$  measurements, offset for clarity, illustrating the reproducibility of the conductance values. The measurements were made with the same MCB but for different retractions/contacts and thus different contact configurations. Offsets of 0.01  $\mu\text{S}$  for the middle curve and 0.02  $\mu\text{S}$  for the top curve are used for clarity. The first step for these three measurements gives values of 22.2, 22.2, and 22.7 megohm (top to bottom); the next step gives values of 12.5, 13.3, and 14.3 megohm. The middle curve is the same data as in (A). (C) An  $I(V)$  and  $G(V)$  measurement illustrating conductance values approximately twice the observed minimum conductance values. Resistances of  $\sim 14$  megohm for the first step and 7.1 megohm (negative bias) and 5 megohm (positive bias) for the second step were measured.

Figures 1 through 4 from Reed et al. 1997.

While the authors do not dwell on the amount of current and whether or not it exceeds or agrees with theoretical expectations, they wish to establish that the observed current flows through a single molecule even though they have no direct means of observing the number of molecules that bridge the electrodes. Their paper is based on four measurements, three of which showing very similar values for maximal resistance or minimal conductance (Fig. 4B and A), while the fourth shows approximately half of the resistance and twice the current flow (Fig. 4C). The first three measurements are taken to establish the high reproducibility of the minimum conductance level which, according to Reed and Tour “implies that the number of active molecules could be as few as one.” While this is, so to speak, the carefully worded official conclusion of their paper, their statistical interpretation of the fourth measurement suggests a stronger claim.

Figure 4C shows [...] measurements of one singular observation that gave resistances that were approximately half (that is, 0.5) the value of the maximum resistances (using averages, 0.63 and 0.45, respectively). This suggests a configuration of two non-interacting self-assembled molecules in parallel, substantiating the idea that the threshold resistance of a single molecule is ~22 megaohm [...] (Reed et al. 1997, 253).

In other words, if one consistently observes a certain amount of current flow and occasionally double that amount, this would seem to confirm the presence of normally one and occasionally two active molecules. In contrast, if there were always anywhere between 5 and 15 active molecules, one would get less consistent results and more smoothly distributed measurements.

What Reed and Tour do not state in this paper, becomes apparent in their June 2000 Scientific American article. Here, the caption of an image of a single benzenedithiol molecule acting as a conductor mentions the “relatively large current flow” (Reed and Tour 2000, 90). They elaborate as follows in the body of the text:

It turned out that the resistance of the molecule was in the range of tens of millions of ohms. The Yale researchers also found that the molecule could sustain a current of about 0.2 microampere at 5 volts – which meant that the molecule could channel through itself roughly a million million ( $10^{12}$ ) electrons per second. The number is impressive – all the more so in light of the fact that the electrons can pass through the molecule only in single file (one at a time). The magnitude of the current was far larger than would be expected from simple calculations of the power dissipated in a molecule [...] (Reed and Tour 2000, 91).

What Reed and Tour call an “impressive” finding has generated incredulity among some of their skeptical peers. To them, the magnitude of the current would indicate that it is not passing through a single molecule. Such a large current, they might argue, would destroy the molecule just as too

large a current will melt a wire. This holds especially for the place of contact where the current is supposed to leave the bulk material and enter a single atom. Reed and Tour recognize this and indicate that their finding is consistent only with a particular account of this process:

The magnitude of the current was far larger than would be expected from simple calculations of the power dissipated in a molecule, leading to the conclusion that the electrons traveled through the molecule without generating heat by interacting or colliding (Reed and Tour 2000, 91).

We are thus confronted with a classical dilemma – indeed, a text-book dilemma for philosophers of science – where one has to either impeach the integrity of an experimental result or revise one's theory, for example by adopting Reed and Tour's somewhat offhanded conjecture.<sup>5</sup> A dilemma like this may well prompt an urgent call for clarification such as Stan Williams's insistence that we must solve the problem of how electrons go through molecules.

All of this adds up to a more or less plausible story about the theoretical interest of Reed and Tour's researches and their perhaps startling conclusion. Indeed, this story would lead one to expect that their papers in *Science* or *Scientific American* might have appeared under the heading "New finding establishes that electrons travel through molecules without interacting or colliding." However, this is not how their researches were presented, received, or discussed by the scientific community.

Stan Williams is a senior researcher for Hewlett Packard. He does not distinguish between molecular electronics and molecular computing but confronts major problems in the pursuit of Moore's law and ever faster, ever smaller computers. He emphasizes that the size-regime of smaller computer chips gives rise to quantum tunneling effects and power leakage, which makes it harder to scale down, leading, for example, to silicon melting. In particular, electron/photon coupling may be responsible for anomalies that need to be understood before he can build the next generation of computers. It is in this context and in view of drastic current changes at low voltages that he calls for an account of how electrons go through molecules (Williams 2002). And this provides the second kind of answer to the question about the nature of Williams's problem, this one belonging to NanoTechnoScience as a place-oriented rather than issue-driven enterprise. Along the same lines,

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5. It is possible, of course, that the dilemma evaporates in light of adequate background knowledge. Mark Reed suggests that "those who seemed surprised by the magnitude had not thought critically about comparing this to the quantum of conductance,  $2e^2/h$ " (personal communication, compare note 10 below). Compare also Di Ventra et al. 2002, 195: "This suggests that molecular wires can operate at very large fields without current-induced breakdown. Also, the molecular device at hand [the one from Reed and Tour's 1997 paper] can carry current densities larger than  $10^9$  A/cm<sup>2</sup>, i.e., much larger than those allowed in conventional interconnects." To be sure, the relevant question of electron transport does not concern simply the current carrying capacity of the molecule but what happens at the place of contact.

when electrical engineer Mark Reed and chemist Jim Tour call “impressive” the number of electrons that pass through their single organic molecule, this is not because of its more or less profound impact on our understanding of nature but because it underwrites their conviction that single molecules can serve as wires in nanoelectronic circuitry. Accordingly, their *Scientific American* article is entitled “Computing with Molecules,” their conclusion that electrons pass through molecules without generating heat appears almost as an afterthought or a mere aside, and the previously quoted caption reads in full:

The relatively large current flow bodes well for the ability of molecular devices to work with more conventional electronics. (Reed and Tour 2000, 90)<sup>6</sup>

### III. FUNDAMENTAL QUESTIONS

While there has been much work on in recent years on molecular conductance and electron transport (Friend and Reed 2004), it does not consist in a debate of theoretically significant claims. It furthers a common project in piecemeal fashion rather than explicitly evaluate a particular position or hypothesis. Prominent candidates for such evaluation would be Reed and Tour’s claim that they measured current passing through a single molecule or their theoretical conclusion that electrons pass through molecules without interacting or colliding. However, skepticism does not issue in a controversy about the Reed-Tour hypothesis with an aim towards its acceptance or rejection by the scientific community at large. Instead, it is deeply embedded or hidden in investigations that actually build upon their researches as, for example, in statements like these:

Pioneering single-molecule experiments were performed by Reed et al. and later by Kergueris et al. The nonlinear current-voltage characteristics (IVs) found by these groups were attributed to the electronic molecular levels. However, several fundamental questions remain unsolved: Are the IVs really arising from transport through single molecules? Is the electronic flow rather wave-like (coherent transport picture), or is a one-by-one electron transport scenario more suitable (hopping picture)? (Weber et al. 2002, 114)

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6. Compare note 10 below. – Jim Tour emphasizes that the high rate of publication recommends the motto “interpretations change while facts remain.” Accordingly, this reconstruction of their work attributes too much deliberate interpretive work to their experimental researches. Tour recounts that a suggestion on the mechanism was requested as a condition of publication by the editors of *Science* for a related paper (personal communication). In this paper, Tour and his collaborators introduced the potential mechanism in a highly qualified manner as “a candidate mechanism.” While they call for further theoretical work, this is justified in strongly application-oriented terms: “Theory to explain the temperature dependencies and future experimental work to examine frequency and optical response should elucidate the transport mechanisms that would further permit engineering of device performance for room-temperature operation.” They add a footnote to this which appears to render this theoretical work redundant: “Since submission of the manuscript, room-temperature [performance] has been observed in a similar molecule” (Chen et al. 1999, 1551).

This statement is taken from the 2002 paper “Electronic Transport through Single Conjugated Molecules” by a research group at the Institute for Nanotechnology of the Forschungszentrum Karlsruhe. The group around physicist Heiko Weber and chemist Marcel Mayor distinguishes itself from its counterparts in the United States by insisting on the fundamental character of these questions, that is, by pursuing molecular electronics as basic research. Their paper therefore begins by duly noting the technological significance of this research as secondary to theoretical considerations.

How does current flow through single organic molecules? This question plays an all-important role in the field of molecular electronics, a field which is not only a fascinating topic of basic research, but may have great potential for future data processing technologies. (Weber et al. 2002, 113)

Clearly, the thesis about NanoTechnoScience as a place-oriented rather than issue-driven enterprise seems to be contradicted by this statement.<sup>7</sup> This paper therefore warrants a more detailed analysis. In particular, one might ask just how it represents basic research in the field of molecular electronics. Closer analysis will show that the Karlsruhe group conceptualizes its research in theoretical terms. It also indicates, however, that this self-understanding remains largely implicit and that the paper constitutes an explicit nanoscientific advance in that the research group is demonstrating the considerable facility it has achieved at handling molecular break junctions experimentally as well as conceptually. Accordingly, their paper offers two versions of its conclusion: the first establishes the conclusion explicitly as a technoscientific contribution to nanoscale research, another flags it implicitly for its possible significance for open-ended theoretical discussion.

A first indication of this balancing act appears immediately after the just quoted opening. While the oldest paper cited by Reed and Tour in 1997 was one of Reed’s first experimental papers on the topic from 1988, Weber et al. follow a 2000 review article in *Nature* and cite “first theoretical considerations” from 1974. However, the considerations in that 1974-article are “theoretical” only in the sense that the authors provided calculations where measurements were not yet available

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7. Indeed, the Karlsruhe group’s emphasis on basic research might also suggest that the thesis of this paper is not about nanoscience at all, but rather about a cultural difference between the pragmatic orientation of nanoscale research in the United States as opposed to the traditional orientation of publically funded research in Germany. Similarly, it could also be a thesis about interdisciplinary collaborations between physics and chemistry in contrast to those between electrical engineering and chemistry. A single case study cannot decide among these various theses. In the end, the notion of place-oriented NanoTechnoScience requires evidence from a variety of sources.



(Aviram and Ratner 1974).<sup>8</sup> Just like the review article from 2000, its horizon of interest does not reach beyond electronic circuitry. Indeed, the review article casts the history of these researches in terms of manipulative access to the nanoscale and to the dictates of Moore's laws:

The first proposals for molecular electronics appeared in the 1970s, but it is only the appearance of a number of scientific and economic developments that has allowed the recent resurgence of activity in this field. Crucial are advances in nanoscale science and technology, such as new fabrication methods and probes, which enable individual molecules or small numbers of molecules to be connected in a controlled manner into actual test devices. The driving force behind this research is clearly the need for suitable alternative technologies to Si-based CMOS, which is expected to reach its limitations in 10-20 years. (Joachim et al. 2000, 547)

Just like the Karlsruhe group, this review article adopts a rather diffident view of Reed and Tour's findings, a view that neither criticizes nor endorses them.

Break junctions involve the gentle fracture of a microfabricated electrode in its centre by mechanical deformation while measuring the resistance of the metallic wire junction. Its application to single molecules is difficult because a liquid evaporation step is required after formation of the junction, and the conformation and the exact number of interconnected molecules remain essentially inaccessible. Nevertheless, measurements have provided estimates of  $R = 22\text{M}\Omega$  ( $T = 5.9 \times 10^{-4}$ ) for a junction containing molecule 9 shown in Fig. 1a. (Joachim et al. 2000, 542-543)<sup>9</sup>

Weber et al. do not cite any discussion, principled considerations, or empirical evidence to explain why Reed and Tour's "pioneering single-molecule experiments" leave them unpersuaded as to whether they really involved single molecules. Their critique of Reed and Tour is only implicit in their own proposal to "unambiguously identify the IVs as current through our sample molecule" (Weber et al. 2002, 114). It serves as further testimony to the ambivalence of the Karlsruhe approach that its theoretical interests are contained in this largely implicit critique, while their own solution to the problem adopts a similar, albeit more persuasive strategy as did their counterparts in the United States.

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8. It calculates  $I$ - $V$  characteristics "of a molecular rectifier including direct electrode to electrode tunneling" which agree rather well with those obtained by Reed and Tour 1997 and by Weber et al. 2002, 118, though it does not anticipate voltages nearly as high. This agreement is communicated visually through the likeness of their diagrams. See Aviram and Ratner 1974, 282, Weber et al. 2002, 116 (Figs. 2 and 3), Reed and Tour 1997, 253, also Di Ventra et al. 2002, 193. This likeness of diagrams may have been the downfall of Jan Henrik Schön who may have taken these diagrams for icons signifying current flow rather than records of particular experimental measurements.

9. Here is another example of an elliptic critique of Reed and Tour: "Due to the lack of any specific experimental information, we assume that a single molecule makes contact to both right and left leads as shown in Fig. 1, even though this configuration might not be the actual experimental one" (Di Ventra et al. 2002, 192). This article goes on to establish a closer fit between (improved) experimental observations and theoretical models.

Weber et al.'s implicit critique of Reed and Tour is that they were guided by the mental model of classical electronic circuitry.<sup>10</sup> Instead of asking a question about nature, Reed and Tour appear to already be designing a molecular computer. They seem less interested in understanding molecules than in forging the smallest possible wire out of a molecule. They were satisfied as soon as they observed an onset of conductance that they could plausibly attribute to the formation of a molecular connection between the electrodes. Accordingly, they didn't consider it necessary to carefully differentiate their observed current flow from the surrounding and initial conditions, for example by investigating bonding configurations and contact geometry<sup>11</sup> or by assessing the contribution of the electric field's bias voltage (Weber et al. 2002, 120-123). Moreover, after they satisfied themselves experimentally that they had obtained a molecular wire, Reed and Tour offer an apparently ad hoc theoretical model for electron transport.

This implicit critique of Reed and Tour by the Karlsruhe group is contained in its adoption of a more principled theoretical stance. Weber and Mayor set out to remedy these deficiencies and thus to improve and amend Reed and Tour's work. They do so experimentally and by modeling the experimental set up. Both parts of their argument advance the same implicit conclusion: While Reed and Tour were interested to show that current was flowing through an individual, i.e., a single molecule, Weber et al. establish that the individuality of the molecule, i.e., the molecule *qua* molecule with a particular shape and structure makes a difference to current flow. In effect, they work towards the non-trivial conclusion that "the chemical [rather than physical] nature of the junction is crucial and predominant for the conductance properties of a metal-molecule-metal junction" (Weber et al. 2002, 124).

Experimentally, the Karlsruhe group advances this conclusion by offering an improved variant of Reed and Tour's experiment. The rather limited statistical interpretation of that original experiment did not exclude the possibility that in all the observations, more than one molecule was active,<sup>12</sup> nor did it offer effective statistical controls (but see Reed and Tour 1997, 253). The paper of the Karlsruhe group is based on a greater number of experimental observations involving two

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10. Compare Michael Gorman's discussion of mental models as a means of structuring nanoscale research (Gorman 2002). Indeed, it is intriguing to ask what mental model is operative in Jim Tour's reminiscence: "Current/voltage responses were recorded for a single molecule bridging the gap. Remarkably, 0.1 microamps current could be recorded through a single molecule. However, few or none of those  $10^{12}$  electrons per second were colliding with the nuclei of the molecule, hence all the heat was dissipated in the contact. Note that the mean free path of an electron in a metal is hundreds of angstroms; hence, it is not surprising that collisions did not take place within the small molecule. Most importantly, since most computing instruments operate on microamps of current, the viability of molecular electronics became all the more tangible" (Tour 2003, 238).

11. "... it becomes evident that the type of bridging as well as the proximity of gold atoms to the molecular  $\pi$ -system has significant influence on the electronic structure and on electron transport" (Weber et al. 2002, 122).

12. In particular, it is hardly credible that their results were based on exactly and no more than four measurements.

molecules that differ mainly in their spatial symmetries. The symmetric molecules produced symmetric current-voltage curves, the asymmetric molecules asymmetric ones, their peak sometimes offset in a positive and sometimes in a negative direction. This affords a more sophisticated version of Reed and Tour's statistical argument. Weber et al. offer 5 observations that, taken together, still "do not give an unequivocal proof, but strongly indicate that we are indeed sensitive to single molecules." In other words, Weber et al. do not claim that their and, by implication, Reed and Tour's molecular junctions do consist of single molecules. They merely argue that their data is statistically sensitive to the individuality of molecules. This is best exemplified by the fourth of their five observations:

For the asymmetric molecule, the spectrum appears either with a peak at  $U \approx -(0.35 \pm 0.1)$  V or a similar peak at positive bias. This discrete asymmetric behaviour indicates that a discrete set of molecules, which is randomly oriented, most probably a single one contributes. A larger set of randomly oriented asymmetric molecules would average out the asymmetry, a fact that has never been observed. (Weber et al. 2002, 118)<sup>13</sup>

The experimental part of the Karlsruhe paper thus appears on the one hand as a mere extension of Reed and Tour's approach. Five years later, one might say, the production and experimental control of molecular junctions has improved. What was once considered a precarious procedure has now been routinized. A greater facility to vary the experiment also provides a regime of improved assessment and control of the experimental observations. This similarity between the two research groups in terms of argument and approach tends to disguise the difference in their orientations. This difference is exemplified firstly by the apparent diffidence of the Karlsruhe researchers as to whether or not they are looking at a wire consisting of a single molecule and secondly by their pronounced interest in the chemical nature of the observed conductance patterns.

An analogous account can be provided for the theoretical part of the Karlsruhe paper. It overtly continues where others leave off. At the same time it questions Reed and Tour's approach by conceptually reframing the issue. Reed and Tour referred to transport models only to show that their findings are physically consistent with physical and chemical background knowledge. In contrast, the Karlsruhe researchers model the onset of conductance in purely quantum chemical terms. Without reference to "elaborate," physically derived "theoretical transport models" (Weber et al. 2002, 124, 123), Weber et al. exhibit the chemical sensitivities of the entire experimental set-up. They model it as a single super-molecule that includes the electrodes as clusters of gold atoms. The

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13. According to Weber (in conversation), the required discrete set of molecules should be no more than a handful, certainly less than ten.

sensitivities of interest are the architectural features of that super-molecule — spatial symmetry, in particular — and the onset of conductivity which moves the molecule from an insulating to a conducting regime.<sup>14</sup>

This difference in approach is underwritten by entirely different, indeed incommensurable ways of using of the term ‘molecule.’ According to chemical usage, a compound of an organic molecule and metal atoms involves complex bonding. Depending on whether ionogenic or covalent bonds prevail, these compounds are referred to as complexes or as molecules (in the case of purely ionogenic bonds one does not customarily speak of molecules at all). In the case of the gold atoms and the organic molecule that serves as the wire, the transfer of charge produces an overlapping of their orbitals. By definition, therefore, covalent bonds prevail in this case and these bonds create a new molecule that includes the gold atoms together with the inserted organic molecule. In these chemical terms, then, one can no longer refer to the (organic) molecule by itself when that molecule shares orbitals with the gold atoms in the transfer of charge. Accordingly, that organic molecule no longer exists as a discrete entity or as a wire that connects the gold atoms of supposedly separate electrodes. By treating the entire experimental set-up as a “supermolecule,” Weber and Mayor follow chemical usage as opposed to Reed and Tour.<sup>15</sup>

No theoretical difference could be greater than that between incommensurable approaches. And yet, the significance of this difference is not reflected at all in the paper by the Karlsruhe group. It implicitly claims, throughout, that the diversity of perspectives advances a common project. It therefore remains unclear even whether the choice of a different conceptualization constitutes a critique of Reed and Tour’s approach. Similarly, the paper by Weber et al. leaves open whether and how their qualitative use of pure quantum chemistry constrains the physical transport models which are, perhaps, too obviously shaped in the image of electronic circuitry.

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14. This transition is marked by the breakdown of the theoretical model that was adopted for an analysis of the insulating regime. "In the insulating regime, no current is flowing and the method [an equilibrium method for investigating the electric field in terms of external electric potentials for the two clusters of gold atoms] is justified to a good approximation. In the conducting regime, different things happen in the experiment and in our model: whereas in the experiment a current is flowing, within our computation the molecule will screen the external potential by a static charge transfer from one gold cluster to the opposite. However, both effects are obviously closely related to conductivity" (Weber et al. 2002, 123).

15. I owe this analysis to Joachim Schummer (in conversation). This case study resonates with Schummer’s contention that any discipline constitutes its objects through its theoretical perspective, its questions, problems and issues. Schummer’s observation raises a skeptical doubt regarding the possibility of a truly interdisciplinary nanoscience. If interdisciplinarity consists primarily in the abandonment, loosening, or black-boxing of the theoretical frameworks of the contributing disciplines, how then is an interdisciplinary nanoscience to arrive at “common objects” (Schummer 2004b, this volume)? Only the development of a specifically nanoscientific theoretical perspective would provide a solution. While George Khushf (2004, this volume) envisions such a new disciplinary perspective, there appears to be little pressure or movement toward its development.

For now, the only explicit conclusion that can be drawn from that single publication of the Karlsruhe group is that they are adding to the conceptual tool-box of molecular electronics (see also Tian et al. 1998, Di Ventra et al. 2002, etc.). Five years after Reed and Tour, researchers have expanded not only their experimental control of the phenomena but also their conceptual grasp. More and more abstract models are becoming available first to represent the phenomena and then to indicate where the phenomenological observations may yet be too crude (Di Ventra et al. 2002, 192-194, Weber et al. 2002, 122).

#### IV. REVISITING THE THESIS

Two distinct attitudes have now been identified, two approaches, perhaps styles of research in molecular electronics. Since one of them implicitly refers to a theoretical conception of basic science, is it really defensible to claim both for the thesis that nanoscale research is a place-oriented technoscience rather than issue-driven science? In conclusion, four considerations are offered in support of this claim.

The endeavor of contrasting the two research groups is caught up in a fundamental difficulty concerning the very notion of "technoscience." This notion was introduced by Bruno Latour (1987) and Donna Haraway (1997) to mark a new stage in the development of science, namely the technological constitution of the objects of scientific research such as transgenic mice that are hybrids of nature and technology. However, as soon as this new era of technoscience was proclaimed, it became possible to consider all of experimental science as technoscience. Even a vacuum-pump or certain observational protocols, one might say, constitute the supposedly natural objects of scientific research technologically. While this appears to dissolve the novelty claimed for technoscience, this claim can be maintained on another level, namely at that of the self-understanding of science (Nordmann 2004b). Perhaps, all science has always been technoscience, but traditionally trained scientists are only abandoning their traditional self-understanding in the contexts of nanoscience, the biomedical sciences and genetics, artificial intelligence research and robotics. Instead of seeking to humbly understand and explain a given nature, they now openly embrace the project of overhauling or transforming nature, of "Shaping the World Atom by Atom" (NSTC 1999, Nordmann 2004a). Thus, the difference between Reed and Tour on the one hand, and the Karlsruhe group on the other hand is not that one has a technoscientific orientation while the other adopts a theoretical stance. Both contribute to NanoTechnoScience. Reed and Tour

do so openly while the Karlsruhe group still represents itself in terms of the traditional opposition between fundamental versus applied science and technology.<sup>16</sup>

Secondly, this paper has shown that the fundamental problem investigated by the Karlsruhe group presented itself not in the development of a quantum-chemical research programme, but in the technoscientific pursuit of electronic circuitry made up of organic molecules. Similarly, their explicit contribution consists in the enhancement of experimental and conceptual control of molecular break junctions. In contrast, their ultimate interest in the specifically chemical nature of this junction appears as an oblique gesture towards an ongoing and open-ended discussion of a fundamental question that stands in the tradition of natural philosophy. Indeed, if their focus had been on theoretical understanding, they could not sustain their implicit claim that incommensurable perspectives can advance a common project. The incommensurability of concepts does not matter precisely because the various perspectives are oriented toward the acknowledged significance of molecular electronics and the interest to achieve electron transport in some kind of circuitry.

Thirdly, this disjunction between the implicit and explicit dimensions of the argument by Weber et al. exposes the missing middle ground. It is significant, I believe, that between the finite demonstration of achievement and an obliquely philosophical gesture there is no overt critical engagement of a hypothesis or theory. Reed and Tour did not place the ball in the court of public opinion. Instead, the ball remained in their court and the scientific community adopted a wait-and-see attitude: "If they think they have mono-molecular-wires, let's see where this gets them; they can win us over by demonstrating a more targeted conceptual, experimental, technical control of the phenomenon. They can present better and better arguments in the form of better and better molecular wires and, ultimately, devices." To be sure, as in any age of exploration and the claiming of new territory, many will not wait and see what Reed and Tour might achieve. Instead, they will themselves attempt to get there first. While such efforts build upon Reed and Tour's experiments, they can do so without buying into or bothering to contradict any particulars of their account. The technoscientific occupation and appropriation of the nanoscale thus differs from standard conceptions of theoretical science not only in the orientation towards its subject-matter but also in the interaction among scientists: The critical aspect or "organized skepticism" of public science takes the backseat to the staking-out and entrenchment of private claims.<sup>17</sup>

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16. This is not to say, of course, that such self-ascriptions are inconsequential for the development of research. To acknowledge this is easy for Kantian, Peircean, or Wittgensteinian philosophers of science, for Weberian or Mertonian sociologists of scientific knowledge. It is far more difficult to acknowledge for all those who are interested in the material culture of (techno)science and therefore tend to deny the historical influence or material efficacy of concepts, ideas, theories, and beliefs.

17. To be sure, Popper's and Merton's view of science as organized skepticism may have become obsolete even before nanoscience came along. The suppression of theoretical disagreement in the advancement of an application oriented research agenda may characterize many scientific publications (compare Carrier 2004). In this case, one might say that nanoscience helps foreground this technoscientific development.

Finally, Joachim Schummer has pointed out that the reasons why experiments are done in chemistry differ from those in physics. They do not serve to test theories or confirm hypotheses. Instead, chemical experiments serve the purposes of “(1) performing chemical reactions in order to form new products [...] (2) investigating various properties of the new products” (Schummer 2004a, 400). While it may appear at first that Reed and Tour’s approach fits this description, the insistence by the Karlsruhe group on an element of basic science points to a middle ground here, too. Research that aims for conceptual as well as physical mastery of a certain territory, domain, or size regime, is interested neither in theory nor merely in novel devices and substances. It is exploratory research, literally speaking, where settlement follows upon exploration and new practices, perhaps a new culture is founded.

## CONTACT

Alfred Nordmann  
Professor of Philosophy  
Technische Universität Darmstadt

nordmann@phil.tu-darmstadt.de

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