Quantum Fantasies and Molecular Realities

Why we should ditch alternative (quantum) computing and instead focus on rethinking molecular science so as to develop full nanotechnology

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Abstract

Quantum computing is criticized as obfuscatory. The problem of an excessive number of continuous parameters is explained by Dyakonov. The origin of the idea of quantum computing (courtesy of Feynman) is investigated - was it just a desperate attempt to circumvent the limitations of computers in the early 1980s? His scepticism is noted as is the astonishing processing power of modern computers. The fundamental problems of quantum computing are set out: it defies basic physics by implicitly requiring sub-atomic control; it cannot be categorized within formal logic; it does not offer true general purpose computing; and, over four decades of work in the field has been fruitless. An alternative research and development objective (again courtesy of Feynman) - namely molecular nanotechnology (MNT) - is set out. The extreme shortcomings of the synthetic techniques of today's material science are described. A brief background to MNT is given, including a summary of the debate between Smalley and Drexler. The simple theoretical resolution to this debate (multitasking) is given and contrasted with single purpose synthetic techniques. The remaining 'causality dilemma' is mentioned. The preferred materials of MNT (diamond and maybe silicon) are contrasted with the molecules of organic chemistry. A novel alternative (by Marson) to self or positional assembly for material synthesis is summarized - namely the directed evolution of mineral nanocrystals by utilizing affinity chromatography and microED technology (in preference to X-ray crystallography). The greater possibilities for self-assembly engendered by tailored nanocrystals are mentioned, as is the most obvious first use of mineral nanocrystals, namely dynamic catalysis.

This paper was originally posted on 31 Dec 2023, had one edit on 2 Jan 2024 (6), and has a few new braced edits (plus an abstract):

Recently {the Department of Industry, Science and Resources (Australia)} announced that applications will be considered for $18.5 million in funding for local 'quantum computing' companies for the purpose of establishing the so-called Australian Centre for Quantum Growth **(1)**. I write this today to make the point that quantum computing is not a worthwhile field of research, that those engaged in it are practising obfuscation in order to win grants, and that there is

no realistic expectation that it will ever yield decent computers {'decent' meaning competitive with classical computers}.

This argument has been made a number of times by those who have investigated the subject, for example physicist Mikhail Dyakonov who said:

Experts estimate that the number of qubits needed for a useful quantum computer, one that could compete with your laptop in solving certain kinds of interesting problems, is between 1,000 and 100,000. So the number of continuous parameters describing the state of such a useful quantum computer at any given moment must be at least 2^1000, which is to say about 10^300. That's a very big number indeed. How big? It is much, much greater than the number of subatomic particles in the observable universe.

To repeat: A useful quantum computer *needs to process a set of continuous parameters that is larger than the number of subatomic particles in the observable universe.* At this point in a description of a possible future technology, a hardheaded engineer loses interest... To my mind, quantum computing researchers should still heed an admonition that IBM physicist Rolf Landauer made decades ago when the field heated up for the first time. He urged proponents of quantum computing to include in their publications a disclaimer along these lines: "This scheme, like all other schemes for quantum computation, relies on speculative technology, does not in its current form take into account all possible sources of noise, unreliability and manufacturing error, and probably will not work." [Emphasis in original] (2)

But one does not need to be a practising theoretical physicist to arrive at such a conclusion. Anyone *objectively* assessing the facts would be sceptical. The idea that quantum computing should be considered a possibility dates back to a speech (and subsequent paper) made by physicist Richard Feynman forty-two years ago, although he *had* previously speculated about it. Feynman was concerned that conventional computers could not effectively simulate molecules and chemical reactions, and he seems to have been sceptical that predicted increases in computer processing power would be of much help in this. In Section 4 of the paper he speculates about developing 'quantum computers' as a way around the problem, but he ends by saying this:

The question is, if we wrote a Hamiltonian which involved only these operators, locally coupled to corresponding operators on the other space-time points,

could we imitate every quantum mechanical system which is discrete and has a finite number of degrees of freedom? I know, almost certainly, that we could do that for any quantum mechanical system which involves Bose particles. I'm not sure whether Fermi particles could be described by such a system. So I leave that open. Well, that's an example of what I meant by a general quantum mechanical simulator. I'm not sure that it's sufficient, because I'm not sure that it takes care of Fermi particles. (3)

Fermi particles - protons, neutrons and electrons - are what everything is made of. Feynman is saying that he is not sure this proposal would work for the one thing he wants to use it for. He could obviously envisage the massive benefits that would flow from being able to take a more systematic approach to designing chemicals and materials at the molecular level, but seems to have been frustrated by living at a time when computers were simply not good enough for the task. This is obvious in hindsight mainly because we can now simulate molecular structures and predict their properties to a level that is far in excess of our ability to physically control them - due to having better computers. Recent notable examples of this include the use of artificial intelligence (AI) - in the form of neural networks - to solve protein folding **(4)** and to identify hundreds of thousands of new materials **(5)**. So clearly Feynman's concerns are out of date - increases in computing power have rendered worries about the limits of 'classical' computing obsolete. And arguably, although Feynman made a great contribution to physics, in the case of quantum computing - due to something akin to desperation - he made a proposal that does not make sense.

He did though feel compelled to give his scepticism the last word - a caution promptly ignored by various researchers eager for the next easy breakthrough (and who as a group have a distinct tendency to hype their work). It would therefore be advisable to list some of the other problems with quantum computing (QC):

- Firstly, it seems to be motivated by magical thinking **(6)**. Computing power has increased since transistors were invented by means of their continued miniaturization. It follows that once we are building computers with molecular scale components, there can be no further improvements (except for those based on design changes). Some people seem to have an ideological objection to that fact, and some of those have become advocates of QC as a result;

- Secondly, QC has no basis in the theory of computing. The data computers process either directly (and approximately) represents some aspect of reality or is a digital simplification of that reality. All computers therefore run on either analog or digital logic, and almost all modern computers are digital devices based on interconnected binary logic gates. In contrast, the earliest computer (the Antikythera mechanism) was analog, as are today's specialized AI chips - although until recently neural networks ran exclusively on digital hardware. But in spite of the all encompassing nature of these categories QC does not really belong to either **(7)**;
- Thirdly, even if they *do* become viable quantum computers can only ever be special purpose devices. As one commentator put it: "**Just a few years until the plastic-bag-full-of-wasps computer achieves supremacy in simulating the behavior of bags full of wasps.**" To head off a broader awareness of such deficiencies QC advocates are often reluctant to explain the details of their prototypes (by providing circuit diagrams for example). Instead they rely on people's incomprehension of quantum mechanics to neuter criticism. But understanding this branch of physics depends above all on an appreciation of the double slit experiment (Feynman said this) and many who do, disagree with QC;
- And fourthly, QC research and development has been a complete failure - its researchers have nothing useful to offer despite over four decades of work. Compare this to every other new computing technology in history, which either worked right away or quickly led to an improved device that worked (they were also often *profitable* right away). QC advocates cannot even describe a path whereby their ideas become viable in theory.

There is no conceivable excuse for a failure of this magnitude, and it would be a tragedy if more public money were to be ploughed into the field. By contrast, developing technologies for arranging the molecular structure of materials (as Feynman ultimately wanted to do) has massive potential. Here is what he said in 1959:

But I am not afraid to consider the final question as to whether, ultimately - in the great future - we can arrange the atoms the way we want; the very atoms, all the way down! What would happen if we could arrange the atoms one by one the way we want them (within reason, of course; you can't put them so that they are chemically unstable, for example).

Up to now, we have been content to dig in the ground to find minerals. We heat them and we do things on a large scale with them, and we hope to get a pure

substance with just so much impurity, and so on. *But we must always accept some atomic arrangement that nature gives us.* We haven't got anything, say, with a "checkerboard" arrangement, with the impurity atoms exactly arranged 1,000 angstroms apart, or in some other particular pattern.

What could we do with layered structures with just the right layers? What would the properties of materials be if we could really arrange the atoms the way we want them? They would be very interesting to investigate theoretically. I can't see exactly what would happen, but I can hardly doubt that when we have some control of the arrangement of things on a small scale we will get an enormously greater range of possible properties that substances can have, and of different things that we can do. [Emphasis added] (8)

Note that the methods today's material scientists have available to synthesize any of the 380,000 newly identified materials mentioned earlier are roughly equivalent to the natural conditions that Feynman implicitly complains about (heat, pressure, and elemental composition). That is to say, it is currently *impossible* {or at least difficult} to synthesize most of those materials, and even when we can synthesize the *unit cell* of a mineral (that arrangement of atoms which, when repeated in a lattice, uniquely defines the material) we have very little control over how *many* unit cells are in a crystal or over the *shape* of crystals (since various shapes are possible with a given number of unit cells). This monumental shortcoming in our abilities is usually completely glossed over when researchers talk about the utility of new materials; but to be fair they have good reason to be reserved. To acquire both that extra control over crystal shape *and* the ability to produce intractable unit cells we would need to try something entirely novel - we would need to develop something equivalent to mechanical engineering and robotics at the molecular level.

A brief background to nanotechnology

This postulated ability is known as nanotechnology - *molecular* nanotechnology to be precise - and simulations of artificial molecular devices do look like engineered components (but with bumps corresponding to individual atoms). Many people have independently concluded that this capability is an inevitable outcome of continued technological progress. But as a BBC documentary put it in the 1990s - it would mean learning to do engineering from scratch. However, in contrast to quantum computing, there has not been much debate over whether molecular nanotechnology is possible. In the one well known debate

from 2001 to 2003, between chemist Richard Smalley and nanotechnology proponent Eric Drexler, Smalley claimed that it could never work because of what he called the “fat fingers” problem. This in essence states that molecular *manipulator* devices are precluded by basic physics because to change function they would need to be structured at a smaller scale than their workpieces - but both would *already* be structured at the minimum *atomic* scale. In response Drexler countered that he had never proposed such a method in the first place.

Fortunately though, the resolution to this dialectic is technically trivial: a molecular device could act on (i.e. alter or move) different molecular structures by exchanging tool heads. This tactic (*multitasking*) is well known to anyone involved in metalworking, or even anyone who merely owns a screwdriver head set. We can also envisage entirely specialized molecular manufacturing devices - resembling factory machines but built at the nanometre scale - so it is not even clear that multitasking is strictly necessary for continued progress in nanotechnology. But regardless of how we classify our techniques, no such system currently exists within inorganic or solid-state chemistry; and they all raise the same question - how do you initially create a system if you need something like that system to create something like itself? Before addressing this conundrum note that molecular manufacturing systems are of fundamental importance to living cells, where a form of molecular multitasking *is* employed (by so-called ribosomes to produce proteins), so at the very least we can be sure that such molecular systems are physically viable.

But both cell metabolism and biochemistry in general fall entirely within the realm of *organic* chemistry; which is the study of carbon based compounds consisting of chains, rings, and branches. Life makes no use of the pure forms (allotropes) of carbon. By contrast, nanotechnology researchers by default use diamond (‘mineral’ carbon) as the working material in their simulations, although silicon *may* be preferable for first generation artificial molecular devices. Note that simulations involving diamond and silicon are performed, and yield good results, using a variant of classical mechanics called molecular mechanics (except when reaction mechanisms are being investigated). This is possible because these materials are intrinsically quite simple to model - compared to proteins for example. However, all molecular simulations depend on making simplifying approximations of continuous functions - only the hydrogen atom can be ‘solved’ perfectly. Nanotechnology researchers therefore obviate

criticism of their simulations by being very conservative in the approximations they use. And consequently, the only *real* criticism of full molecular nanotechnology is that we do not know how to bring it about. But is the challenge really that difficult?

How to develop nanotechnology

Emulating the conditions present in nature (heat, pressure, and elemental composition) does allow us to synthesize various materials but, as touched on earlier, it does not give us anywhere near enough control. Typically, if such a synthesis is tailored to produce nanometre scale crystals, it results in a range of mineral species. These may differ by mass, electric charge, or structure. The first two of these qualities allow for the separation of different species using conventional physical or chemical techniques (e.g. chromatography). The third quality presents a more subtle challenge - we are talking about species (*structural isomers*) which differ only by shape. If we could separate mineral species by this criterion we would be able to direct the evolution of minerals (and synthesize a variety of otherwise unobtainable structures) by iterating phases of crystal growth, isomer separation, and mineral species identification **(9)**. And fortunately there is a well established technique (*affinity chromatography*) for separating molecules on the basis of their structure - it works by exposing mixtures of chemicals to antibody proteins, which are then separated according to *their* physical properties. A given antibody protein will of course selectively latch on to antigens with a particular molecular structure - that's a big part of how the immune system works. They would therefore be perfect for separating isomers in inorganic chemistry, but strangely this possibility is not mentioned in a handbook on the subject I acquired a few years ago. After crystal growth and isomer separation we would determine the structure of each mineral species, select the most convenient, and then use *its* crystals to seed the next iteration (and repeat as many times as necessary).

I mention this proposal here because I would not criticise an attempt to solve a problem without first attempting to come up with a better solution. It is easy to see why Feynman was fascinated by the possibility of gaining more control over the structure of materials. One of the first things we could do if we were able to make small arbitrary crystals (of carbon or silicon) would be to add functional groups to them and join different crystals together with single covalent bonds. These composite crystals could form molecular devices with moving parts - and

could thereby act as catalysts. Note that {most} of the catalysts in living organisms (i.e. enzyme proteins) have internal moving parts, whereas none of those in synthetic chemistry do. Introducing internally dynamic *mineral* catalysts to synthetic chemistry could significantly improve the yield and efficiency of chemical reactions - without us having to deal with the complications of using enzymes. For example: a better version of the Haber-Bosch process would allow the current technique (which consumes large quantities of natural gas) to be phased out; and improved methods for making fuel (e.g. kerosene) directly from carbon dioxide in the air could eventually put the global oil industry out of business. And once we have built simple molecular devices why not build more complex ones? And why not then move on from directed evolution to directed synthesis and build devices to be used for making other molecular devices?

This kind of research offers a steady stream of real-world applications; and it could commence with relatively little initial funding because much of the necessary equipment is already available. For example, the mineral species identification phase will only be practical if the most powerful form of microscopy, namely microcrystal electron diffraction (microED), is used. But fortunately, various research groups in Australia can already do that type of work. {The main concern should be} to see that public money is spent in a way that yields the best outcome.

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