Molecular Nanotechnology – the Best Tech on Offer (if only we could find the assembly manual)

Version 2 ▪ Mark C Marson ▪ 1 Aug 2025

Abstract

I here address a problem which is preventing the development of full molecular nanotechnology (MNT) defined as the ability to exactly arrange the molecular structure of materials – in particular those made of crystalline carbon or silicon. I ask where technological progress is leading and argue that the ability to synthesize any viable material is the only final objective that makes sense. I give a brief account of how this idea developed from the 1950s on and recount one notable debate which illustrates both the fundamental difference between MNT and regular technology and a potential obstacle to the development of MNT if we adhere to conventional approaches. **I then describe a novel synthetic method that solves this problem – the directed evolution of nanomineral isomers – and detail its six main steps: nanomineral growth, antibody-nanomineral association, antibody differentiation, antibody-nanomineral separation, nanomineral characterization and/or selection, and iteration.** I discuss nanomineral catalysis and the augmentation of nanominerals with functional groups, the nature of the design process for nanomineral components, a few other obvious applications of MNT, the potential of so-called smart materials, and the implications of MNT for medicine and robotics. In conclusion I argue that the development of MNT is essential for fulfilling our potential as a civilization, and that if we want to keep progressing we will need to exploit a much greater range of inorganic materials (just as nature has exploited a huge range of organic chemicals).

Introduction – an overview of technology

The most distinctive feature of humanity is our use of technology, which can be defined as the extension of our abilities resulting from our control over matter. Indeed, the major historical epochs – the stone, copper, bronze, and iron ages – are named after the predominant hardware material of the time. Our technology evolved for millennia, but progress sped up in the seventeenth century, due in part to the emergence of modern science. Our tools had allowed us to study natural and artificial phenomena more carefully, which led to theories explaining how the physical world works, which in turn often inspired and enabled the development of even better technology. This prompts an obvious question: how will the process end? Is there an ultimate technological capability which, if acquired, would enable us to do anything that is physically and economically possible? And if so, how do we manifest it? That is to say: is there anything stopping us from improving today's technology up to the limits set by physical law? Our metalworking abilities, which contemporary engineering is based on, are limited only by the skill with which we can shape and blend the metallic elements (perhaps with supplements like carbon) but such technology is ill suited to helping us set out structures below a certain size. Meanwhile, the capabilities of our molecular technologies (chemistry and biochemistry) are determined by how effectively we, or the micro-organisms we control, can synthesize organic molecules. But these *latter* disciplines leave an enormous range of potential molecular technologies unexplored and undeveloped – those are technologies that could exist if we were able to specify the molecular structure of minerals and the shape of mineral particles at the nanometre scale.

This is the realm of inorganic chemistry and material science. Each type of mineral is defined by its 'unit cell' – an irreducible arrangement of atoms conceptually similar to a chemical compound – and these usually have distinct isomeric forms (i.e. *crystal polymorphs*). When the geological preconditions necessary for a particular mineral are present, a lattice of its unit cells will grow and a crystal is formed. (This can be contrasted with metal alloys. Whereas alloys also have predefined proportions of elements, unlike minerals they do not consist of repeated unit cells. This means that the atomic arrangement and elemental proportions within a small piece of alloy are not set exactly and that the applicability of its structural identity – as substitutional or interstitial – is dependent on which elements are close to the atom under consideration.) We can emulate geological processes in the laboratory with the right equipment, but we cannot synthesize arbitrary chemically stable mineral unit cells which do not have preconditions that correspond to easily adjustable parameters. This matters because it has become clear that we can apply the methodology of mechanical engineering to the design of nanominerals. As things stand then **a truly vast range of materials and molecular devices – which we know are viable – are physically unobtainable.** Speaking figuratively, almost half of the technological possibilities that molecular science promises (i.e. those based on minerals not organic chemicals) are simply not available to us.

Molecular Nanotechnology – the last and best technology

The field of molecular nanotechnology consists of the study of those technological possibilities and the development of techniques to synthesize atomically tailored minerals. MNT was inspired, to a certain extent, by the emergence of biochemistry in the first half of the twentieth century and the resultant realization that some types of macromolecule within the cell *are* actual molecular machines (which transport molecules and ions and perform chemical reactions); a fact which almost guarantees that molecular engineering more broadly can be implemented in various other ways. The most famous exposition of this was Richard Feynman's speech **There's Plenty of Room at the Bottom**(1) given in 1959, quote: "The biological example of writing information on a small scale has inspired me to think of something that should be possible. Biology is not simply writing information; it is doing something about it …" Feynman then talked about practical ways to miniaturize contemporary technology, but went on to talk about the potential of tailored minerals (which would be the end result of such miniaturization) expressing confidence that "we will get an enormously greater range of possible properties that substances can have, and of different things that we can do." He came to this conclusion: "Ultimately, we can do chemical synthesis. A chemist comes to us and says, "Look, I want a molecule that has the atoms arranged thus and so; make me that molecule." … But it is interesting that it would be, in principle, possible (I think) for a physicist to synthesize any chemical substance that the chemist writes down. Give the orders and the physicist synthesizes it. How? Put the atoms down where the chemist says, and so you make the substance."

Feynman gave a follow-up talk titled **Tiny Machines**(2) twenty five years later in 1984 and (if we collate his thoughts on the matter) it is apparent that he came painfully close to explicitly stating that inorganic molecular machines would be able to carry out reactions in organic chemistry. It is also clear that his idea of performing *organic* reactions using conscious positioning is unrealistic – surely we would use artificial enzymes of some kind? The idea that we might "Put the atoms down" – while still inaccurate – is a better description of how some *inorganic* materials might be synthesized by inorganic molecular machines. Basically though he was saying that the 'tiny machines' would be able to make almost anything, a position that various people would arrive at independently over the years (before the internet made that unlikely). The general concept was fleshed out a few years later by Eric Drexler in his book **Engines of Creation**(3), and soon after that Drexler and Ralph Merkle used computer simulation to confirm that nanominerals could *in theory* be assembled to form molecular devices. If we *could* develop efficient techniques for making and assembling arbitrary nanominerals as theorized it would represent the final phase of the era of miniaturization. It would also, for the first time, offer the defining benefit of digital computing to conventional engineers (as opposed to chemists or biochemists): the ability to make a perfect copy of something without the need to worry about precision.

However, as alluded to earlier, it is not clear that we can develop MNT simply by improving existing synthetic techniques – if we imagine where those could lead on their own we run into a wall far short of being able to build inorganic molecular devices. If we want to break through that wall we must first determine what concepts from conventional engineering are applicable in

MNT and then clarify our aims accordingly. We also need to acknowledge a basic axiom: a technology can only be *first* developed with *pre-existing* tools. The best engineering tool we have ever possessed is the human hand, and it would be nice if we were able to manipulate atoms and molecules freely and bond them together exactly as we wished (within the rules of chemistry) as if playing with building blocks – but unfortunately reality is not that convenient. Everything at the molecular level is structured to the same atomic level of detail. Consequently, for any given molecular structure there is one and only one spatially complementary structure that can hold it perfectly and thus manipulate it with perfect control (enzymes are a good example of this – the most efficient are tailored to catalyze one reaction only). MNT researchers would not therefore be able to build a *single* 'molecular assembler' that could make anything else, because that would entail the manipulator changing *its own* structure. This point was made – implicitly – by chemist Richard Smalley in a debate with Drexler from 2001 through 2003(4).

There is however a very simple remedy for this problem – multitasking. A common design solution in engineering is for each tool in a set to be attached to the same type of grip. A compatible machine can then pick up and use all of the tools with one gripping mechanism. (Note that every interaction in this scenario is entirely specialized.) This tactic is used in machine tool multitaskers, multi-bit screwdriver sets, and ribosomes – although ribosomes do not 'pick up' tRNA molecules, rather they select them from aqueous solution using complementary hydrogen bond patterns on mRNA strands, and the workpiece (i.e. the protein) folds into shape by itself so the ribosome does not have to move around it. Multitaskers will certainly play an important role in later generations of MNT, but it is difficult to see how that prospect can help us create MNT in the first place since the simplest way to build a molecular multitasker would be with the help of another molecular multitasker! (This 'chicken or egg' dilemma could be seen as Smalley's underlying criticism; see Ref 4.) Note too that anything that can be made with a multitasker, either macroscopic or molecular, can also be made using a single purpose method – that is why the constituent machines of production lines are usually single purpose. To state the obvious though we do not have molecular scale nanomineral production lines either – so the problem persists. To solve it we need to stop thinking about final forms and instead think about the incremental steps we can take to eventually attain them.

Directed Evolution – a remedy for the intractable

An obvious parallel to this situation exists in the natural world where species evolve through incremental changes in their anatomy or physiology, which would both be associated with genetic changes. (Notably, the most important parts of ribosomes are composed of RNA, which presumably would have been subject to natural selection before nucleic DNA – according to the theory – took over that role.) But could such a strategy be applicable outside biology? A nanomineral can be imagined as a single atom onto which other atoms have been added at the right places in a certain order so that a new nanomineral isomer is formed – this is how we would build a model of such a structure in computer simulation. (The term 'isomer' is used to emphasize the fact that two nanominerals could have the same *chemical* composition but different *structures*.) However, if we try to adapt the 'chemistry by fiat' approach of molecular simulation in order to do synthesis in the real world, we immediately find that – as mentioned above – we would need a variety of molecular tools to do the job. Those are tools we simply do not possess; so if we really want to atomically tailor minerals we have no choice but to first grow a *variety* of nanominerals without regard to the isomeric forms they take(5). Following this we would obviously need to *select* the nanominerals we want from the inevitable isomeric mixtures and build on those chosen variants to obtain improved isomeric nanomineral molecules. The crucial point is that this process of variation and selection could be iterated to facilitate *cumulative* improvement. (The selection would be done using a technique called *affinity chromatography* in which assorted antibody proteins are employed to do their usual job of selectively latching on to diverse molecular shapes.) More detail on how this would work is given below, but in terms of broad strategy we would be temporarily setting aside conventional methods in favour of a *directed evolutionary* approach using artificial selection.

To begin with here are a few preliminary observations about the pros and cons of directed evolution (in this context) compared with general chemistry and evolution in nature. Starting with the cons: the main drawback of this method is that it would suffer from very low overall yield – however, to compensate we could simply start off with more precursor. One *potential* drawback arises from the fact that a variety of distinct synthetic pathways might be available for obtaining a given nanomineral – this means that to get a satisfactory yield it might be necessary to get different pathways to converge at a later iteration of the synthetic procedure. As for the pros: the most obvious advantage of directed evolution is that it would lack the aimlessness of biological evolution. It could be compared to retrosynthetic analysis in organic chemistry where researchers have a target molecule in mind and make a plan in reverse by choosing plausible precursors until they arrive at easily available chemicals. Another, partially related, advantage is that it would be much faster than biological evolution. In nature gene pools are often stable for many generations before a new mutation is selected for as beneficial and spreads; with directed evolution we would be selecting a novel variant from each *successive* generation. Here is how the procedure would work in detail:

1. **Nanomineral growth:** A pure nanomineral sample would be exposed to growth conditions for a short duration – these would typically be high temperature, high pressure, or laser irradiation. By having a sufficiently short growth period we could ensure that the resulting nanomineral variants (NMVs) were only marginally larger than their precursor. The NMVs could then be augmented with polar groups to ensure their solubility in water;
2. **Antibody-nanomineral association:** The resulting mixture of NMVs would be exposed to a range of antibodies in aqueous solution (as in normal affinity chromatography) – each matching antibody species would then weakly bond to an unspecified but *structurally* specific NMV. This 'random fitting' precludes any need to simulate or make predictions about antibody bonding with the iteration's desired NMV;
3. **Antibody differentiation:** The antibody-nanomineral complexes would be separated from eachother by exploiting differences in the mass or charge of their *antibodies* e.g. using conventional chromatography. We thus avoid the problem of how to separate NMVs with different structures but *the same* mass and charge (i.e. different isomers). This is why affinity chromatography is so well suited to this kind of work;
4. **Antibody-nanomineral separation:** Each fraction from Step 3 would have its antibodies separated from their *isomeric* NMV (iNMV) molecules using conventional chemical techniques. To get the best result from Steps 2 through 5 each active antibody species would have to bond to one iNMV only and vice versa, but if this did not happen at first (see Step 5) different antibody combinations could be tried until this *was* the case;
5. **Nanomineral characterization and/or selection:** The structure of each iNMV would be determined using x-ray diffraction or micro-electron diffraction(6). At this step we could also find out if a fraction was both pure and adequate (i.e. if its antibody was both selective and sufficiently effective) and thus decide whether or not to continue the trial. Assuming fraction purity and adequacy we would select the iNMV which was the best intermediate for eventually obtaining the target nanomineral; and,
6. **Iteration:** The intermediate iNMV thus chosen would be put through Steps 1 through 5 again to obtain the next desired iNMV. This would be repeated as many times as necessary to obtain the final desired nanomineral product. Note that we would soon know which species of antibody to use in each iteration so as to effectively extract the correct iNMV, thus reducing Steps 2 through 5 to a simple extraction procedure.

Note that before commencing such research we would need to choose the initial experimental material – basic considerations restrict this choice to silicon based minerals or the hard mineral form of carbon i.e. diamond (which is considered inorganic even though it is made of carbon). In Version 1 of this paper (**MNTBTO1, 14 April 2022**) I had doubted the wisdom of using nanodiamonds to get the project started – even though diamond is in general ideal for MNT. However, I now think that nanodiamonds *would* be a better choice than silicon for the initial material. My opinion changed after looking into two subjects: the difficulties of working with silicon(7) and advances in the synthesis of nanodiamonds(8). This investigation also affirmed **MNTBTO1's** take on the importance of the functionalization of nanodiamond isomers (for reasons other than making them water soluble) indeed chemists seem to have an enduring fascination with this topic(9). Note that nanodiamond functionalization, in addition to having obvious applications in organic chemistry, may also in time provide a more efficient way to make tailored nanodiamonds themselves than the method set out in this paper(10). Obviously this should be one of the main goals of MNT research since the very low yields of directed evolution, even if manageable, *would* be best avoided. But remember that even if superseded the directed evolution method can be kept in reserve to fill in any gaps in our future synthetic capabilities.

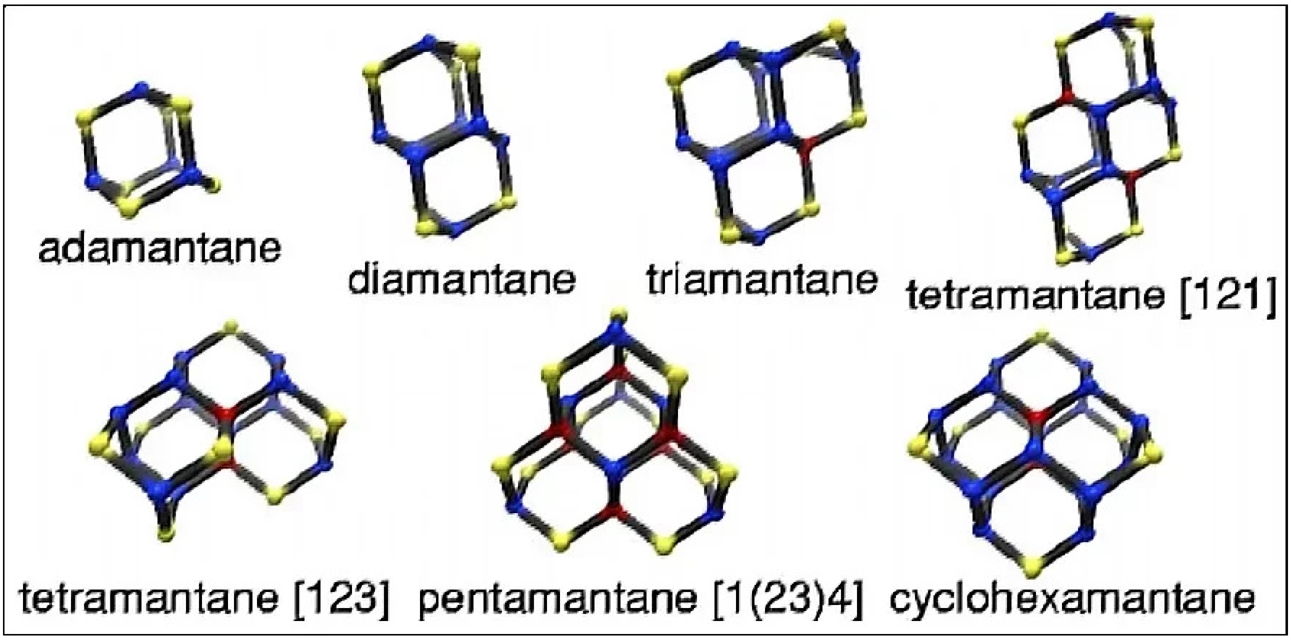

Figure 1: Some nanodiamond minerals; tetramantane shows isomeric variation.

To summarize then: we can in general incrementally improve the molecular structure of a given nanomineral by directing its evolution using artificial selection; this would be more direct and quicker than evolution in nature; nanodiamonds could be our working material from start to finish; and crucially, we do not require positional control of nanominerals (i.e. nanodiamonds) beforehand in order to work toward that as a goal.

Applications of Molecular Nanotechnology

The incentive for developing MNT is the wealth of practical applications it promises. Most obviously, tailored nanodiamond molecules could be used to catalyze reactions in organic chemistry; and this ability would be enhanced if, in addition to using the surfaces of nanodiamonds for immobilization, we assembled whole nanodiamond molecules into devices with moving parts which were able to 'grab' molecules and pull them apart or 'hold' reagents and push them together. This is analogous to how many enzymes work, although for them the reaction is almost always coupled with the metabolizing of ATP. So how could a nanodiamond be incorporated into a molecular device as a moving part? Normally in mechanical devices the parts hold eachother in place, but it would be difficult to assemble that kind of structure in the early stages of MNT, so instead we could use the flexibility and rotatability of some chemical bonds to add internal dynamics to composite nanodiamond devices.

To begin with we would augment a nanodiamond sample with special surface bonded functional groups (see **Ref 9**); the resulting mixture could then be separated into variant specific fractions based on *where* exactly on the surfaces those groups had bonded. Different nanodiamonds functionalized in this way would react together in solution according to normal chemical rules, which would allow us to join two nanodiamond molecules with a single covalent bond, and as a rule such a joint structure would have predictable dynamics around that bond. So if a way could be found to momentarily 'refold' the subunits in relation to eachother – perhaps using laser irradiation or electroactive polymers – it could catalyze a reaction between immobilized reagents. (This strategy of connecting subunits to form macromolecules is conceptually similar to various biochemical processes e.g. how amino acids are linked using peptide bonds in protein synthesis or the way proteins use disulfide bonds to stabilize their tertiary structures.) Some techniques in industrial chemistry, such as the Haber process, could be significantly improved using dynamic nanodiamond catalysis, and it would allow other reactions to be commercialized for the first time e.g. the conversion of carbon dioxide and water into ethene (non-IUPAC: ethylene) and the various reactions needed to completely recycle plastic.

All such catalysts would of course have to be designed on computer before we tried to build them(11). Fortunately though the computational methods for simulating nanodiamond devices are simpler than those for simulating proteins (protein folding is innately complex) and we could facilitate the design process by employing virtual reality – this would allow researchers to 'get a feel' for the nanodiamonds, making the task more similar to the kind of tinkering inventors have always made use of to refine their ideas. Eventually, we could arrange nanodiamond catalysts in production lines so that a workpiece molecule could be passed from one to the next until we had a completed product. This could be very efficient but would require specialized apparatus for handling the workpiece together with a way to position each device in the correct place – nothing indicates that such molecular manufacturing systems would be unviable though. Five more obvious applications of MNT are: the ultimate miniaturization of computer circuitry (and circuits which are assembled not etched); direct brain-computer interfacing; more convenient chemical testing and separation techniques (even for very similar substances like rare earth metals); better growth media and scaffolds for cultured meat; and, novel drugs that make use of the rigidity of nanodiamonds to interact with biomolecules in unique ways (this is already being done at an elementary level).

But we can easily envisage even more sophisticated applications for MNT, because nothing would be stopping us from combining molecular machines into complex self-contained entities i.e. nanobots. Such a development would erode the distinction between machines and the materials they are made from, because why not use nanobots themselves as a material? A 'smart material' consisting of a mass of nanobots could be programmed to form certain shapes or behave in certain ways when experiencing particular environmental conditions. This would enable the self-assembly of a wide range of structures at all levels of complexity – everything from bricks to artificial organs to diffuse 'utility fogs' which could easily transition to their solid phase. Entirely independent nanobots would also have valuable applications – they could, for example, move through the bloodstream and deliver drugs precisely where required or possibly even perform something equivalent to surgery on individual cells. They could also be designed to emulate and/or work with biological cells. Neuron-like nanobots, for example, could integrate into the brain and amplify our abilities or heal brain damage. Being able to assemble artificial organs serviced by circulatory nanobots would in turn enable the creation of entire artificial organisms. We could, for example, build gardening robots able to precisely administer nutrients or deal with pests – organic farming would thereby become easier and cheaper than modern chemically assisted farming. Indeed, MNT could facilitate the creation of a range of artificial but lifelike machines equipped with sensors and tools and able to do all sorts of jobs under a wide variety of environmental conditions.

Conclusion

Clearly the development of molecular nanotechnology will have wide ranging consequences, as one might expect from a technology that would enable us to synthesize any chemically viable material. If this sounds excessively optimistic note that all rigorous computer simulations (i.e. those done with conservative physical assumptions) attest to MNT being possible. The only serious criticism of MNT which has persisted – that no one can explain how the technology could *initially* be created – is cleared up by this paper. ▪ In addition to the applications given above MNT is a prerequisite for the successful exploration of space, not only because of the wealth of new materials it would offer, but also because it would allow a myriad of 'industrial' processes to be carried out by tiny molecular machines (which could be produced in any amount necessary without difficulty). Indeed, a complete self-replicating nanobot 'industrial complex' could be the size of a protozoan. Furthermore, each copy of a nanobot would be an exact molecular replica of the original so successive generations would not suffer from any degradation over time (quality control would therefore be unnecessary). The kind of comprehensive self-reliance this would offer would make MNT indispensable for so-called Von Neumann probes – the autonomous spacecraft intended to travel to other solar systems before replicating and sending off their own progeny. ▪ We could start moving forward by carrying out a proof-of-concept test of directed nanomineral evolution. This would be followed by creating nanodiamond catalysts for organic chemistry, before creating nanodiamond devices for synthesizing other nanodiamonds. Up to now we have picked the low hanging fruit of material science (e.g. glasses, ceramics, and metals) while chemical synthesis has been largely concerned with the standard forms of *organic* chemistry – polymers, rings, branches, functional groups, and ligands. But for technological progress to continue we need a more *general* ability to synthesize nanomineral molecules (particularly those of diamond); then *both* divisions of the molecular realm can be exploited to the full.

NB The main change made to the paper in Version 2 concerns the initial experimental material – see Page 7, Directed Evolution section, and **Refs 7** & **8**. Edits have been made throughout for readability. No AI was used in copy-editing any version of this paper.

Acknowledgements

Many thanks to Professor Ross Barnard at University of Queensland who made me aware of affinity chromatography in 2015, at which time it was apparently only used for organic chemistry. Title image by David Zydd.

References

(1) **p3 There's Plenty of Room at the Bottom; Richard Feynman; 1959;** https://www.zyvex.com/nanotech/feynman.html**:**

> 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.

(2) **p3 Tiny Machines; Richard Feynman; 1984; Muon Ray** https://www.youtube.com/watch?v=4eRCygdW—c&t=0s**.** Feynman says this about molecular scale machines (26:33):

> But I said that this talk was about machines and of course a computer is a kind of machine, but the machine you usually [associate with the word] is machines with movable parts. Now let us talk about the possibility of making machines of movable parts which are very tiny – the immediate look in all the faces [says] what for? Mental entertainment. Maybe someday they'll find a use for it okay. How small can we make machines? It's just thinking for the fun of it okay. Don't worry about it that [it] hasn't any application. It doesn't cost you anything not to have an application. It's just fun okay so we're not going to worry about how we use these dumb things we're just going to try to make them. How could we make movable matter, little machines, tiny machines that would operate that are very very small?

He goes on to discuss a 'top down' approach to building such machines which can be contrasted with the 'bottom up' approach advocated in this paper. Scanning tunnelling microscopy or molecular scale electronic patterning (perhaps utilizing tetracyanoplatinate salt crystals) might offer ways to integrate the two approaches.

(3) **p3 Engines of Creation: The Coming Era of Nanotechnology; K Eric Drexler; 1986; ISBN 0-385-19973-2.**

(4) **p4 Richard Smalley and K Eric Drexler; 2001-03;** https://en.wikipedia.org/wiki/Drexler%E2%80%93Smalley_debate_on_molecular_nanotechnology**.** In the initial Scientific American article Smalley wrote:

> Because the fingers of a manipulator arm must themselves be made out of atoms, they have a certain irreducible size. There just isn't enough room in the nanometer-size reaction

> region to accommodate all the fingers of all the manipulators necessary to have complete control of the chemistry … [Also] the atoms of the manipulator hands will adhere to the atom that is being moved. So it will often be impossible to release this minuscule building block in precisely the right spot. Both these problems are fundamental, and neither can be avoided. Self-replicating, mechanical nanobots are simply not possible in our world.

to which Drexler replied:

> This ubiquitous biological molecular assembler [the ribosome] suffers from neither the "fat finger" nor the "sticky finger" problem. If, as Smalley argues, both problems are "fundamental", then why would they prevent the development of mechanical assemblers and not biological assemblers? If the class of molecular structures known as proteins can be synthesized using positional techniques, then why would we expect there to be no other classes of molecular structures that can be synthesized using positional techniques?

Drexler is using a rather broad definition of the word 'positional' here ('ordered' might be better) but proteins do demonstrate control of molecular structure in three dimensions so his scepticism about that being unachievable is warranted. Later he said:

> The impossibility of "Smalley fingers" has raised no concern in the research community because these fingers solve no problems and thus appear in no proposals. Your reliance on this straw-man attack might lead a thoughtful observer to suspect that no one has identified a valid criticism of my work. For this I should, perhaps, thank you.

Of course, it is possible that Smalley was not familiar enough with biochemistry (or metalworking) and so lacked the experience necessary to appreciate Drexler's point. But saying that a thing that performs many actions cannot exist is only one step away from simply opting for many things to perform many actions, and so the theoretical objection to MNT resolves itself without further effort.

(5) **p5 Synthesis of Higher Diamondoids and Implications for Their Formation in Petroleum; Dahl, Moldowan and Wei *et al;* 2010; Angewandte Chemie.** This paper sets out the problems conventional chemistry has with synthesizing nanodiamonds (in any kind of controlled manner) in explicit fashion:

> The mechanism for formation of these nanodiamonds for a long time was attributed to thermodynamically controlled carbocation rearrangements. Such mechanisms enable the practical synthesis of [diamondoids with up to three adamantane cages] but they fail in the production of the higher diamondoids. A detailed analysis of the mechanism for adamantane formation from a single starting material shows an amazing 2897 pathways; a more limited analysis of triamantane formation through carbocation pathways indicates at least 300 000 potential intermediates. Prospects for higher diamondoid syntheses by these pathways are bleak due to a lack of large polycyclic precursors, problems with intermediates trapped in local energy minima, disproportionation reactions leading to side products, and the exploding numbers of isomers as the size of target higher diamondoid products increases. With the failure of syntheses of higher diamondoids through carbocation rearrangements, attempts at their preparation were abandoned in the 1980s.

MNTBTO is an attempt to deal with "the exploding numbers of isomers as the size of target higher diamondoid products increases" which is seen as the most serious problem of those listed. I first noted directed evolution using antibodies as a potential solution to this problem in 2011, quite possibly in response to reading the here referenced paper; for the full solution though I did require one additional innovation (see **Ref 6**) and a greater awareness of the relevant synthetic techniques (see **Ref 8**).

(6) **p6 'A new day for chemistry': Molecular CT scan could dramatically speed drug discovery; Robert F Service; 2018;** https://www.sciencemag.org/news/2018/10/new-day-chemistry-molecular-ct-scan-could-dramatically-speed-drug-discovery**:**

In chemistry, structure rules because it determines how a molecule behaves. But the two standard ways to map the structure of small organic molecules … have drawbacks. This week, two research teams report they've adapted a third technique, commonly used to chart much larger proteins, to determine the precise shape of small organic molecules. The new technique works with vanishingly small samples, is blazing [sic] fast, and is surprisingly easy … Instead of firing their electron beam from one direction at a static crystal, they rotated the crystal and tracked how the diffraction pattern changed. Instead of a single image, they got what was more like [a] molecular computerized tomography scan. That enabled them to get structures from crystals one-billionth the size of those needed for x-ray crystallography.

(7) **p7 On the Potential of Silicon as a Building Block for Life; Petkowski, Bains and Seager; 2020;** https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7345352**.**

(8) **p7 Nanodiamonds: Synthesis, properties, and applications in medicine; Qin, Yang and Lv *et al*; 2021; Materials and Design** https://www.sciencedirect.com/science/article/pii/S0264127521006468**:**

Yang *et al* used laser ablation of graphite targets in water to synthesize diamonds, and the thermodynamics of ablation of graphite targets in water, acetone, and ethanol to synthesize NDs has also been studied [in 2007]. The synthesis of NDs by laser ablation is actually based on the interaction of a laser-generated cavitation bubble with a solid boundary, which facilitates the nucleation, growth, and solidification of the nanoparticles under the fast quenching conditions. Wang *et al* prepared NDs by bombarding graphite targets in water with laser irradiation and proposed the kinetic principle of diamond formation [in 2005]. NDs can be synthesized by laser ablation at room temperature, and the preparation efficiency is ideal. In addition, because of the reaction in the liquid phase, impurities are not easy to intervene [sic]. But its disadvantage lies in the high consumption of energy and low productivity.

Being able to grow nanodiamonds in aqueous solution makes the growth step of directed evolution significantly more convenient. However, when we want to develop a better method for *controlled* nanodiamond synthesis we will have to come up with a way of removing *chosen* surface hydrogens before substituting carbon groups (see **Ref 10**).

(9) **p7 Diamonds are a Chemist's Best Friend: Diamondoid Chemistry Beyond Adamantane; Schwertfeger, Fokin and Schreiner; 2008; Angewandte Chemie** https://www.researchgate.net/publication/216574201**:**

Adamantane chemistry has been studied and reviewed very extensively in the last 50 years … These amino derivatives are important compounds in terms of further functionalization, especially for the preparation of peptides. The best counterparts for a peptide bond are arguably carboxylic acids. These diamantane carboxylic acids, their methyl esters, acyl chlorides, acetic acids derivatives, and their bromine- or hydroxy-substituted derivatives have been prepared and studied very intensively by various groups in the past few years.

Arguably, the ideas in **MNTBTO** are a natural extension of such work; after all, how useful will nanodiamonds ever be in medicine if we disregard isomerism?

(10) **p7** We can imagine what form such improved nanodiamond synthesis methods will take by extrapolating from the ideas in this paper. Here is one attempt at a 'post-evolutionary' nanodiamond synthetic procedure template:

a) Design a varied set of specially functionalized nanodiamond components amenable to controlled chemical assembly;
b) Synthesize the nanodiamond components and assemble them in aqueous solution to form various *nanodiamond catalyzing devices* (NCDs);
c) Transfer the NCDs to reaction chambers to be immobilized in such a way that their reactions can be electrically powered in place;
d) Replace the medium in the reaction chambers with an inert gas (e.g. argon) before introducing supplementary reagent molecules in aerosol form;
e) Move the workpiece nanodiamonds successively from one chamber to the next as aerosols;
f) In each chamber each NCD would attract a workpiece and a reagent molecule to its reaction site using complementary charge patterns; and,
g) Each NCD would be electrically powered (see Step c) to then remove the appropriate surface hydrogen (this is called *hydrogen desorption*) from the workpiece before adding a carbon group sourced from the reagent molecule at that site.

Note that if such an approach is to enable a more general ability to synthesize nanodiamonds it will be necessary for those later NCDs to be focused solely on the surfaces they are intended to modify (i.e. the charge patterns in Step f would be for the reagents only); holding the workpiece nanodiamonds in place would have to be done using specialized grips (perhaps reminiscent of the clay templates hypothesized in the clay-abiogenesis theory of the origin of life). But considering that such grips would have to be able to hold 'any' molecular structure – and would therefore have to be similarly varied themselves – how would we manufacture them? The obvious answer would be to use proteins as the grips – assuming that we can design or evolve them so that they maintain their specialized gripping abilities when removed from aqueous solution.

(11) **p8** Note that software for doing molecular design work is freely available (see https://www.samson-connect.net/) and whereas designing nanodiamond devices may not strictly require artificial intelligence – because the needed structure should follow from properly specifying the function – material science more generally is already making use of it. See **This new AI creates ANY material you want; AI Search; 2025;** https://www.youtube.com/watch?v=7_y9aF_T9qc which covers **A generative model for inorganic materials design; Zeni, Pinsler and Zugner *et al*; 2025;** https://www.nature.com/articles/s41586-025-08628-5**.** Here is part of the paper's abstract:

> [MatterGen] can further be fine-tuned to steer the generation towards a broad range of property constraints. Compared to prior generative models, structures produced by MatterGen are more than twice as likely to be novel and stable, and more than 10 times closer to the local energy minimum. After fine-tuning, MatterGen successfully generates stable, novel materials with desired chemistry, symmetry, as well as mechanical, electronic and magnetic properties. As a proof of concept, we synthesize one of the generated structures and measure its property value to be within 20 % of our target. We believe that the quality of generated materials and the breadth of MatterGen’s capabilities represent a major advancement towards creating a foundational generative model for materials design.

Numerous comments from the YouTube video's comment section echo the motivation behind **Molecular Nanotechnology: the Best Tech on Offer**:

Sounds like this comes up with goals; now we need something that comes up with the path to achieve those new goals, the process to manufacture the materials in bulk. **@tiagotiagot**

[The] issue is synthesizing, any chemist can come up with the necessary structure and function... **@MrPyro91**

I feel one of the best uses for this kind of AI would be one that knows what our current manufacturing capabilities are. Given the materials we have and manufacturing technologies we have I am betting the AI would be able to find other materials that we CAN make with existing infrastructure that "no one thought about before". New and novel materials, even though [they] might have all the things requested, just might not be manufacturable with current readily available equipment or knowledge. **@daveland2653**

We could try to get [AI] to create the models to assemble atoms together to create any material. We would still have to figure out how to build a machine that could actually perform the process of assembling atoms but imagine the possibilities. **@gtrguy17**

Does it only produce material designs [for which] we have evidence we would be capable of producing them? Or can you bias it for designs that we are likely to be able to synthesize? There was one crystal lattice with multiple elements in there that I would be very surprised if we were capable of manufacturing it in a lab, let alone at scale. **@DustinRodriguez1_0**

This AI can find atom configurations for new materials with desired qualities, but it seems it does not tell us how to produce these materials. So if I get the formula $TaCr_2O_6$ I might need to do more than melting Ta and Cr under the influence of Oxygen to bring all the atoms into the right order within the [crystalline] structure. Does the AI take into account that some materials configure [almost] by themself e.g. [Bronze] by mixing and melting Cu and Sn, but others even if made only from a single chemical element are not easy to make. An example is Graphene. The people who first made Graphene found a (not very efficient) method almost by accident. If, before Graphene was known, an AI told us to form hexagonal layers of carbon atoms, we had no idea to make it. **@thomasschmidt9264**

Now we need a company that can synthesize (create [in] real life) any material that MatterGen can generate. And then we need 3D printers than can [3D] print with whatever materials that MatterGen can generate [100 & Fire emojis] **@OrbitalVibes**

Does it tell you how to make the material? Can it cost optimize yet? **@tristan7216**

I mean, are we even able to produce these materials? Discovering a theoretical material is one thing, but producing it cheaply and at scale is a feat of its own. For instance, we've known about nanotubes for decades now, but it's still not available to the average person **@jonahbranch5625**

Could this be used to make any material in real life? **@Srindal4657**

It's good, but useless if the found material can't be practically produced. **@FernandoGarcia-hc9mn**

… Some generative AI [designs] some bizarre material in the digital mathematics world, doesn't mean anyone anywhere is ever going to be able to figure out how to turn it into something. Is it news worth hearing about? Yes[.] Is it a big deal going forward? Maybe, to even probably. Will that reward be seen in this decade? Almost certainly not. How about the next decade? Maybe … **@1450JackCade**