

# Homo Citans and Carbon Allotropes: For an Ethics of Citation

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allotropy · carbon · citation ethics ·  
publication practices

Dedicated to Gene Garfield

## On the Shoulders of Giants

In a classic of scholarship, “On the Shoulders of Giants,”<sup>[1]</sup> Robert K. Merton, a great sociologist of science, traces the involuted history of a remark by Isaac Newton, “If I have seen further it is by standing on ye shoulders of Giants.” Merton’s book is also a humanist romp, a deliciously humorous dissection of scholarly pretensions, including his own.

Merton follows The Aphorism, as he labels this apposite expression, back to Bernard of Chartres. And he documents its passage through a menagerie of more or less illustrious Gallic, Jewish, and Anglo-Saxon writers, to Newton, and past him to Claude Bernard, Bukharin, and Freud. Each should have cited the source of that seductive simile. Some did, some made up imaginary sources. Still others just tried to pass the expression off as their own creation, deigning citation unimportant.

Meanwhile, The Aphorism kept its hold. Because it packages in a physical metaphor a truth: Even when we imagine (and want others to acknowledge) that our piece of hard-won knowledge is novel, better, or deeper than that which came before, we know that in fact it depends on what others have done previously. The novelist’s citations are

hidden, for PhD students to disinter. The scientist (male and female) is perforce and explicitly *homo citans et citatus*.

This essay will first take a look at the reasons why appropriate citation is essential to the well-being of our profession. It will then pass from ideals to two case studies of failures in citation in one subfield of chemistry and physics, that of hypothetical carbon allotropes.<sup>[2,3]</sup> One of these cases has managed in three decades to accumulate an intricacy that took eight centuries for The Aphorism. Fault finding is easy; we will try to move beyond it in two ways. First, by giving down-to-earth suggestions for more-effective literature searching, and even advice on what to do if, God forbid, you should be guilty of omitting a crucial citation. And second, by introducing, at least in the specific subfield we discuss, a computer-age tool for avoiding making a fool of yourself.

## Why we cite

The reasons are numerous; here is a selection.

1. *The tradition of scholarship.* To mix similes, if not dwarves on the shoulders of giants, we are links in a chain. Citation is natural, as old as the laziness that is most often behind the failure to give credit where credit is due. European, African, and Asian scholarly cultures have left us with a tradition. This is worth upholding, and not just in Anatevka. Take a look the citation-studded orthography of a page of the Talmud (redacted 600 CE),<sup>[4]</sup> or Confucius (551–479 BC), which cites the older texts of the Shangshu (Shu-ching, Book of Documents),<sup>[5]</sup> and you will see the scholarly chain displayed. Anthony Grafton, in his delicious book, “The Footnote: A Curious History,” traces the evolution of referencing in European historical scholarship from the Renaissance onwards.<sup>[6]</sup>

2. *History.* Yes, there are new things in this world—a gram of buckminsterfullerene, special relativity. But everything, absolutely everything, even the molecule and theory named, has antecedents. Reserving ethical considerations for a separate category, we are unabashedly and persistently curious about how the new came about. Knowledge is received, and we respect that.

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3. *Utility.* In our scientific papers we use measurements by others. We also use definitions, concepts, and techniques. It is inefficient to repeat the calorimetry that determined the heat released in the burning of, say, 10 g of ethanol, or to rehearse the computation of the average position of an electron in a many-electron atom. So we cite the NIST Chemistry WebBook, an electronic resource maintained by the National Institute of Standards and Technology (which in turn cites and compares critically several experimental measurements of the heat of formation of ethanol).<sup>[7]</sup> Or we put in a reference to Desclaux's classic tables of atomic calculations.<sup>[8]</sup>

4. *Avoidance of duplication.* We cite so we should not, need not, repeat unnecessarily what was done before. We wish to avoid duplication. Mind you, experimental measurements and computer proofs alike need checking. As we write this, there is a report of superconductivity at 200 K in a material ever-present in the chemistry labs of yore, hydrogen sulfide. You can be sure the experiment is being repeated in several laboratories; it's hard to do so, quite a different story from cuprate superconductors. The vaunted reproducibility of scientific measurements needs to be probed; none of this hurts the scientific method.<sup>[9]</sup>

Is the ninth synthesis of palau'amine publishable? Of course it will be, if done by a different route than the first such synthesis or is otherwise distinguished. Is the design of a carbon allotrope, claimed to be unprecedented, publishable if there is a previous paper on the same allotrope already in the literature? This is going to be a point in the two detailed case studies we will present. But we do not evade judgment: No, unless the second paper adds value to the design, say by calculating some property.

5. *Establishing credentials.* We cite so that our fellow chemists see that we know the literature. This is to establish the ground on which our discovery or insight may be seen as new or an advance in understanding. Crank papers are recognizable by their lack of citations, or by obsessive self-citation. A synthesis of taxol that does not cite Robert A. Holton's first synthesis of the molecule<sup>[10]</sup> is not likely to be published. Citing the other eight syntheses listed in the Wikipedia on the synthesis lists puts us into the grey area of the too little/just enough/too much citation.

By the time a good graduate student has written his or her PhD thesis, they can predict 90% of the references in a paper published on the subject of that thesis. Which is little consolation when that paper is not by themselves.

6. *Priority.* We also cite others (and our previous work) to establish our own research as innovative, as different from what had been done previously.

Danger lurks here. Even as there is a natural tendency to doubt our own powers or originality (are we speaking about ourselves?), observation of human nature seems to point in another direction: people tend to exaggerate the quality of what they have done. We hate those papers whose authors think that the way to establish their own claims to originality is by downgrading the partial understanding that came before, citing errors, omissions, all that went wrong. The psychology is transparent: when you have little to say, you begin by pointing out what other people got wrong. When you really have

something new to say, you never do this, you just launch into what you have done.

Yet priority is important. It might seem that questions of priority shouldn't be of concern to "science"; if Einstein had not derived in 1905 the equation  $E = mc^2$ , surely someone else would have gotten it soon thereafter.<sup>[11]</sup> Or not so soon. But this is a psychologically uninformed view for two reasons. First, given the paltry financial rewards of most scientific research, the ideas we have and the molecules we make are our "mind children". As such, they are priceless. And if someone does not cite them, it feels like a violation.<sup>[12]</sup> Second, the truths we glean, the molecules we make, are universal. But our world is shaped by individuals creating the new. And they do so through interacting with each other in a certain chronology. The world is changed by hazard and circumstance. If Kekulé had not given us the structure of benzene 150 years ago, organic chemistry might have gone in a different direction, emphasizing molecules and reactions different from those that have shaped our chemical experience.

Establishing priority is important. Especially so when utility, attested to through commercial value, enters the picture. The rewards are all that money can buy. Recognition of priority here is through the patent system, a legal fiat to exploit an invention in exchange for revealing it. Unfortunately, we do not have the space and time here to probe the fascinating logic of priority and citation in patents, and the practice of "examining" patents, so as to find prior art.

Patents aside, the meaning of discovery is sometimes complex. We direct the reader to the fascinating history of the discovery and patenting of lasers,<sup>[13]</sup> and to the story of the discovery of oxygen, the subject of a play by Carl Djerassi and Roald Hoffmann.<sup>[14]</sup>

7. *Negotiating the "anxiety of influence".* This category follows hard on the previous one. The term is taken from Harold Bloom's remarkable book,<sup>[15]</sup> and we are grateful to Mario Biagioli for reminding us of it.<sup>[16]</sup> We are a walking congeries of influences—of our parents, our teachers, the papers we have read. And somehow out of this patchwork of influences, aided by the workings of chance, we make the new: a molecule that in fact was not on earth before, a new theory. How can we be original, when so much went into what we do?

Harold Bloom saw this tension as being most explicit in poets, for their forte was their originality. This is perhaps not that different from scientists. Bloom worked out a typology of strategies used by poets, explicit and subconscious, for denying, evading, and generally finding ways around the influence of other poets. These categories make for good reading, for one can see point-by-point parallels in them to the experience of contemporary chemists.

What citations do for chemists is to allow them to negotiate the anxiety of influence. We cite work that piecewise precedes ours, we name the pieces, factual or conceptual, that enter what we do. Admittedly, quite selectively, and occasionally this gets us into trouble. The web of the 50-odd citations of a typical chemical paper reveals the influences, and at the same times serves to assuage the underlying doubts of the author about the originality of the work.

8. *Connecting up the world.* It's wonderful to see an organic synthesis marked not only by a brilliant plan (or a brilliant salvage job once the initial plan went awry), but also the pulling into use of a variety of synthetic methodologies that are scattered here and there across the literature. And for a theoretician, what a pleasure to have a way of thinking explain two or more puzzling problems, ones that no one would think of associating. R. B. Woodward talks of this in his Cope Lecture,<sup>[17]</sup> and it is what made Roald Hoffmann devote his Nobel lecture to the isolobal analogy<sup>[18]</sup> and not the history of orbital symmetry control of organic reactions.

9. *Fairness.* Such an old-fashioned concept, some might say. And is it not moored in the hypocritical class structure of colonial gentlemen? No, fairness is important. Ultimately, we cite to be fair. To acknowledge the achievements of those who came before. Behind this is an ideal, unvoiced, a shared conception of a body of reliable scientific knowledge built by many individual contributions. And a delight, in a troubled world, that there is a place where things are approximately as they should be. Science is a micro-society, and it was Merton who delineated for us how this society differs from others. One of its fundamental obligations (and satisfactions) is that one give credit where credit is due. As Mario Biagioli suggested to us, science is also a commons; citations are part of the fees one pays to use it.

### What Our Journals Say

The American Chemical Society has a set of Ethical Guidelines to Publication of Chemical Research.<sup>[19]</sup> On the subject of citation, these read:

*"An author should cite those publications that have been influential in determining the nature of the reported work and that will guide the reader quickly to the earlier work that is essential for understanding the present investigation. Except in a review, citation of work that will not be referred to in the reported research should be minimized. An author is obligated to perform a literature search to find, and then cite, the original publications that describe closely related work. For critical materials used in the work, proper citation to sources should also be made when these were supplied by a nonauthor."*

The European Association for Chemical and Molecular Sciences, in its "Ethical Guidelines for Publication in Journals and Reviews",<sup>[20]</sup> writes:

*"Authors have the following responsibilities:*

*3.1 To gather and interpret data in an honest way. Editors, referees, readers and publishers have the right to assume that submitted (and published) manuscripts do not contain scientific dishonesty and/or fraud comprising among others fictitious data, plagiarized material, reference omissions, false priority statements, "hidden" multiple publication of the same data and incorrect authorship.*

*3.3 To give due recognition to published work relating to their submitted manuscript by way of correct reference and citation. All sources should be disclosed, and if a significant amount of other people's material is to be used, permission must be sought by the author in accordance with copyright law."*

The Council of Science Editors (CSE) published in 2006 and revised in 2012 a "White Paper on Promoting Integrity in Scientific Journal Publications".<sup>[21]</sup> The feeling we get on reading its 81 pages is of CSE "running scared." As far as citations go, it has a whole section on citation manipulation, but good citation practice is mentioned only two times, as far as we can see:

*"The reviewer should ensure that an observation or argument that has been previously reported be accompanied by a relevant citation and should immediately alert the editor when he or she becomes aware of duplicate publication.*

*...editors should require authors to 'Cite and reference other relevant published work on which the submitted work is based.'"*

These are good statements, but overall, the White Paper is disappointing. Codes and guidelines serve many functions: Even as we know that human beings may violate them, we set out in them ideal (yet realistic) norms. They certainly serve as more or less legalistic standards in case of violation, but they also have a moral and exhortatory purpose. We think it is as important to show young people in our profession what is right and good as it is to draw lines, prescribing violations.

We wish our journals would say more. Actually, the ethics of citation is one place where the time-honored journal peer review process does well. Scientists are people, and people are people, which means that they are lazy, even as they are decent. Roald Hoffmann has looked carefully at unrefereed papers, such as those in arXiv<sup>[22]</sup> (a repository of electronic preprints not taken to by chemists, but used widely by physicists, astronomers, and others). To him, these papers are often deficient in the quality of their illustrations and the fairness and adequacy of the way they cite the literature. We posit that this is not done maliciously, just out of laziness. In a well-refereed journal, the reviewers enter the context of criticism. It is their business to find fault, often to our annoyance when it is our papers that are being reviewed. If the referees are properly chosen—it is the editors' métier to do this—then this is where reviewers shine. They tell us of work we have missed, of work to which we should have given more credit. They keep up the ethics of citation. And they also get the authors to improve their drawings.

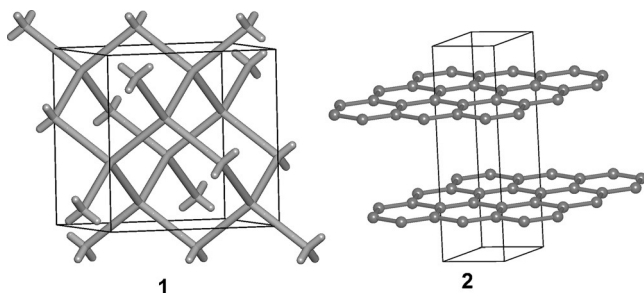
Use engenders abuse, that is the human condition. Most citation sins are of omission, but there are some of commission. We avoid explicit discussion of scientific misconduct, fraud, and plagiarism.<sup>[23]</sup> This is not because we are unaware of them, and not because they are unimportant. It's just that we don't want to be distracted from showing why citation really matters, and helping people to improve their citation practice. Yet, as Harriet Zuckerman wrote to us,<sup>[24]</sup> it's not a bad thing to remind scientists of these blights upon our profession, and their apparently growing incidence.

If citation is our subject, it is especially important that we bring to the reader a selection of previous thought on the subject. To show, among other things, how unoriginal we are... This we will do, but it's time to move to some specific illustrations. We then return eventually to the literature on citation practice and ethics.



## Carbon allotropes

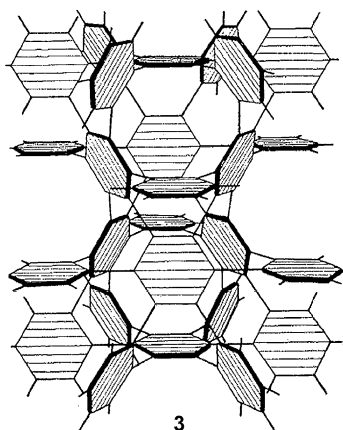
We are going to look at hypothetical structures for arguably the most important chemical element, carbon. Diamond and graphite have been known for millennia, but it is only 100 years ago that we learned (from single-crystal X-ray diffraction) the structure and metrics of cubic diamond (1)<sup>[25]</sup> and graphite (2), at roughly the same time.<sup>[26]</sup> Graphite is known in hexagonal and Bernal forms, which correspond to different stacking of what are now called graphene layers. Hexagonal diamond, or lonsdaleite, was established some years later, although its existence has been recently questioned.<sup>[27]</sup>



It became clear early on, at least on paper, that diamond and graphite are really the first members of a family of polytypes. The small dispersion energies involved in the aggregation of graphene layers imply a variety of stacking modes: AA, AB, ABC, and so on. For diamond, strong as the bonds between what we perceive as horizontal cyclohexanoid sheets are (part of that is an illusion created by our inability to integrate layers and true tetrahedral symmetry—there are chair cyclohexane rings, but no distinct axial and equatorial bonds in cubic diamond), one can also envisage polytypes. Lonsdaleite is the first in an infinite series. SiC makes them real, with a vengeance.

Humanity's incendiary proclivities have no limit. So all along we have had a variety of pyrolytic carbon materials that resist structure determination. Out of a study of one of these, in what is perhaps the first suggestion of a hypothetical carbon allotrope, came H. L. Riley's 1946 structure 3.<sup>[28]</sup>

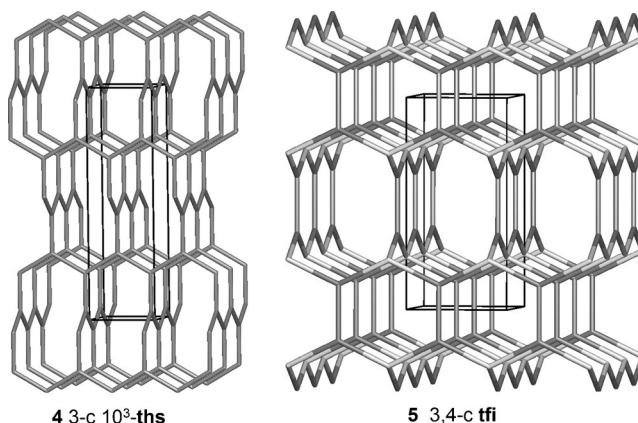
Structure 3 is clearly low in density and relatively unstrained. Riley's carbon, subsequently named "polyben-



zene,"<sup>[29]</sup> will not have a chance against diamond at high pressure. But one day, chemists will find a clever way to make it at ambient pressure.

Next in the roll of real allotropes came buckminsterfullerene. It was initially a gleam in theoreticians' eyes (none of whom cite each other),<sup>[30]</sup> sadly ignored, and then discovered for real in gas-phase carbon-ablation studies<sup>[31]</sup> and eventually synthesized in bulk.<sup>[32]</sup> Now relatively cheap, the molecule, which is thermodynamically unstable but kinetically very persistent, has become a wonderful nexus of chemistry and physics. And of course, there is a family of larger and equally persistent fullerenes, as well as nanotubes.

With no disrespect towards fullerenes, let us restrict ourselves to 3-dimensional infinite networks of elemental carbon. One of us (Roald Hoffmann)<sup>[33]</sup> and Ivan V. Stankevich<sup>[34]</sup> separately began to think about carbon allotropes in the early 1980s. We show here two structures the Hoffmann group came up with: 4<sup>[33]</sup> (with Tim Hughbanks, Miklos Kertesz, and Peter Bird) and 5<sup>[35]</sup> (with Mike Bucknum; further work on 3,4-connected nets with Ken Merz, Sandy Balaban).<sup>[36]</sup> Where available, we provide bold three-letter symbols for nets (as suggested by M. O'Keeffe)<sup>[37]</sup>, here **ths** and **tfi**, respectively. **tfi** stands for three-four-#i, and there are also **tfa**, **tfb** and so on. Both **ths** and **tfi** have been observed in many coordination networks. The nets in structures 1, 2, 3 are called **dia**, **hcb**, **pbz**, respectively.



As plane-wave-based calculations of extended systems became easy to do, the flood gates opened, so to speak. Computational chemistry and physics at an intermediate level has always been easier than experiment. We have counted several hundred papers suggesting "new" carbon allotropes. We put "new" in quotations, because, as we will show, many are repeats. And the titles of the papers that describe them don't stop with "new" or "novel"; enhancers such as "super-hard", "remarkably stable", and "viable" abound. Let us not get into what is at work here, namely hype.<sup>[38]</sup>

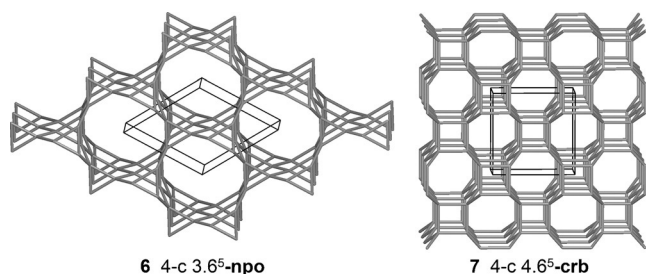
We introduce next the first of two detailed case studies of citation amnesia in the field of carbon allotropes. We do so with trepidation, since the terminology of this subfield of solid-state chemistry quickly grows arcane. Given the sad compartmentalization of our molecular science, the extension in three dimensions of what on close examination are no more

than the simplest organic building blocks, coupled with the nomenclature of networks, builds up in no time the kind of complexity that makes our mind cloud over. We know that this is so, and apologize to the reader for subjecting him or her to the detail necessary to establish our case (or Merton's in "On the Shoulders of Giants"). You will be forgiven if you skim over the next section.

### Davide's story

In August 2014, while working on building a database on carbon allotropes, DMP came across a paper in *Phys. Rev. Lett.* proposing a three-dimensional elemental carbon kagome lattice (CKL) and the structurally related interpenetrated graphene network (IGN).<sup>[39]</sup> The authors did not report the coordinates—unfortunately this tendency is quite common in the literature of hypothetical carbon allotropes, which makes the results quite difficult to reproduce—but only the unit cell and some bond lengths. Nonetheless it was evident that the reported 4-connected net was the same as one called hcp-C3, which was reported in 1999 by P. A. Schultz, K. Leung and E. B. Stechel from Sandia National Laboratories.<sup>[40]</sup>

This net with small 3-rings was later observed in the zeolite nitridophosphate-1 and called NPO,<sup>[41]</sup> hence the net name **npo** in the RCSR database (6). Digging deeper, we found that **npo** was reported in 1992 as net 36 in Figure 2 by M. O'Keeffe in his enumeration of uninodal nets with 3-rings,<sup>[42]</sup> which refers back to J. V. Smith in 1979 (net 94 in his Figure 7),<sup>[43]</sup> both reported as already described by A. F. Wells in 1977 (Figs 9.15a and 9.16 of the remarkable Wells book).<sup>[44]</sup>



The story just begins here. In 2003, **npo** is described as a hexagonal sphere packing 4/3/h3 by Sowa, Koch, and Fischer in their ongoing research on the complete derivation of all homogeneous sphere packing, which was started in the seventies.<sup>[45]</sup> More recently, **npo** was re-examined as hcp-C3 in 2012.<sup>[46]</sup> Furthermore, the structurally related IGN (see above) can be traced to a net called 3,4-**bik**-Cmcm<sup>[47]</sup> and had been reported as ZGM-12.<sup>[48,49]</sup> Indeed the work on CKL and IGN focuses on properties not studied in the previous report on hcp-C3 and ZGM-12, but nonetheless, previous reports describing these structures should have been cited.

But no one is safe in this field, for many networks were known before their re-discovery as carbon allotropes; in fact in the cited 1999 paper on hcp-C3, a body-centered tetragonal allotrope with 4-rings was reported as bct-C4. Electronic bibliographic searching of the literature was harder then, and

so P. A. Schultz, K. Leung, and E. B. Stechel also missed that the same net was reported earlier by R. H. Baughman and D. S. Galvao,<sup>[50]</sup> there called 8-tetra(2,2)tubulane, and was mentioned a few years later again by the same group, now calling it R<sub>2</sub>.<sup>[51]</sup>

What's in a name? The same net has also been called "rectangulated carbon",<sup>[52]</sup> with proper reference to the Baughman works; simply "D",<sup>[53]</sup> with no references except to A. F. Wells seminal works (see below); and (2,2) I4/mmm(2),<sup>[54]</sup> with no specific reference.

After a few years of silence, an important experimental study on cold-compressed graphite<sup>[55]</sup> stirred the theoretical community to action, and the structure reappeared twice in 2010: in March as bct-C<sub>4</sub>, a "viable sp<sup>3</sup> carbon",<sup>[56]</sup> with reference to the 1999 Schultz paper, and in October as plain "bct-carbon" with the laconic sentence "This structure appears to be similar to that found in previous studies" referring to the 1999 Schultz and 2004 Strong papers.<sup>[57]</sup> A veritable torrent of papers followed, recomputing the same structures (together with other hypothetical ones) and calculating all kind of properties,<sup>[58-68]</sup> without citing the older references. The earlier work of Baughman was acknowledged, together with Umemoto 2012, only in two papers.<sup>[69]</sup> Three other publications cited the 1999 Schultz paper.<sup>[70]</sup>

Only one group, that of E. A. Belenkov, has carefully collected all references and atomic coordinates in a book<sup>[71]</sup> and several papers.<sup>[72]</sup> They used the nomenclature LA3 for bct-C<sub>4</sub> and TB for **npo**.

Moving to more chemical literature, it is easy to find that the network of bct-C<sub>4</sub> is known as **crb** (7; the boron framework of CrB<sub>4</sub> and related compounds).<sup>[73,74]</sup> In 1988, it was proposed as a tetragonal carbon net by J. K. Burdett and E. Canadell.<sup>[75]</sup> But the net was known much earlier to the great structural chemist A. F. Wells; one finds it in his 1954 second paper of the series "The Geometrical Basis of Crystal Chemistry." There it is called Net 7 and illustrated in his Figure 6.<sup>[76]</sup> In 1971, W. Fischer in his search for tetragonal sphere packing shows **crb** as 4/4/t5 in his Figure 4.<sup>[77]</sup> And the zeolite expert J. V. Smith called it net 3.<sup>[78]</sup> In 1977, Wells reported **crb** as (4.6<sup>5</sup>)-a in his book<sup>[44]</sup>, together with **npo**, and in the paragraph dedicated to nets with point symbol<sup>[79]</sup> *m.n*<sup>5</sup> writes:

"The nets 3.6<sup>5</sup> and 4.6<sup>5</sup> are particularly closely related, since they consist of "cylindrical" tunnels on the walls of which the plane 6-gon net is inscribed, three tunnels being linked by 3-gons in 3.6<sup>5</sup> and four by 4-gons in 4.6<sup>5</sup>. The latter represents the arrangement of B atoms in CrB<sub>4</sub> [our **crb**] and 3.6<sup>5</sup> [our **npo**] correspond to the positions of the centers of the spheres in the open sphere packing 4<sub>2</sub> (hexagonal variant) of Heesch and Laves..."<sup>[80]</sup>

Both nets are drawn as projections in Figure 9.15 and as stereopictures of handmade models in the Wells reference Figures 9.16 and 9.17. The latter 4<sub>2</sub> sphere packing **npo** is also illustrated in the cited 1954 Wells paper as a packing of tetrahedra in Figure 17. Like **npo**, **crb** was found as the underlying net for a body-centered tetragonal tectosilicate with the zeolite name BCT.

Some final comments. As should be crystal-clear to anyone in the field, if you think up a new net, you'd be well

advised to look for it in Wells.<sup>[44,81]</sup> And/or in more recent collections like RCSR [Ref. [37]]. More on nets could be found in Ref. [82]; for the use of net collections in the search of allotropes see Ref. [83].<sup>[82,83]</sup> The story we have elaborated also resembles one told a few years ago<sup>[84]</sup> about another hypothetical carbon allotrope, this time a 3-connected one called **srs**.

We also note, sadly, that the original older papers are much less cited/remembered than the two that stirred the field in 2010. The citations collected to date are: 23 for 1993 Baughman et al.<sup>[50]</sup> and 25 for 1999 Schultz et al.,<sup>[40]</sup> while 2010 Umemoto et al.<sup>[56]</sup> has 124 citations and 2010 Zhou et al.<sup>[57]</sup> has 60. This is not Merton's "obliteration by incorporation", it's something else.

To summarize: Not quite Bernard of Chartres, but Heesch and Laves in 1933 (3.6<sup>5</sup>-**npo**) and Wells in 1954 (4.6<sup>5</sup>-**crb**).

### Citations for citation

There is another case that we wish to put before you, but let us return first to citation practice. We have no pretensions to being original in delineating the reasons why we cite. The practice of citation itself is very old, as we've mentioned. Science came to citation late, its practices borrowed from established modes of scholarly argument in literature, religious dispute, and legal practice.

Once, there were guides to good citation practice. Here is what Jacques Barzun and Henry Graff write in the 5th Edition of "The Modern Researcher" (the first edition, in 1957, had the same words):

*"Though the researcher is never entirely free from the necessity of accounting for his words through footnotes, it is not the writer who determines the number and fullness of these notes, but the subject at hand and the presumable audience. To the extent that footnotes communicate a part of the meaning and attest reliability, they are as important as any other part of the work. Hence an author should develop judgment about when and what to footnote.*

*All quotations that are more than passing phrases or anonymous remarks require a footnote. So do all novel or startling assertions and all distinct elements in a demonstration or argument. Beyond this. A good rule is to write a note whenever you think an alert person might feel curiosity about the source of your remarks.*"<sup>[85]</sup>

Barzun and Graff's book, directed primarily at humanities scholarship, has a full, readable chapter on "The Rules of Citing." From which the above quotation is drawn.

More directly aimed at scientists is E. Bright Wilson's 1952 advice in his "An Introduction to Scientific Research":

*"Ample references are important in order to enable the reader to obtain the immediate historical background of the problem and any previous attempts to solve it. References should also be given to more complete descriptions of the apparatus used or to descriptions of the apparatus or method from which the present one was evolved. Any outside data, facts, equations, or arguments employed should be supported by references. Finally, papers reaching similar or opposed conclusions should be listed..."*

*...In the whole matter of credit to others, including a proper perspective of the background in the introduction, references throughout the text, and credit at the end, a generous attitude is the most effective one from a purely selfish viewpoint. Scientists form one group which is practically never deceived by men who push themselves forward on the work of others. Failure to give proper credit to another's work can generate more bitterness than any other action.*"<sup>[86]</sup>

A National Academies pamphlet "On Being a Scientist: Responsible Conduct in Research," now in its 3rd Edition, has a very nice section on Sharing of Research Results. It says in part:

*"Once results are published, they can be freely used by other researchers to extend knowledge. But until the results are so widely known and familiar that they have become common knowledge, people who use them are obliged to recognize the discoverer by means of citations. In this way, researchers are rewarded by the recognition of their peers for making results public..."*

*Citations are important in interpreting the novelty and significance of a paper, and they must be prepared carefully. Researchers have a responsibility to search the literature thoroughly and to cite prior work accurately. Implied in this responsibility is that authors should strive to cite (and read) the original paper rather than (or in addition to) a more recent paper or review article that relies on the earlier article.*"<sup>[87]</sup>

In 2010, DMP with Blatov and O'Keeffe wrote a paper on nomenclature for nets.<sup>[79]</sup> This work has been quoted more than 300 times, but quite often using the wrong nomenclature, the one that we tried to teach people to forget. The paper was cited, but clearly not read. Simkin and Roychowdhury come up with a way of estimating from a stochastic model the percentage of citations actually read by the authors; it is a discouragingly low number.<sup>[88]</sup>

At the 2nd World Conference on Research Integrity, Singapore, July 22–24, 2010, a position statement was developed on "Responsible research publication: international standards for authors." It has a few (too few in our opinion) items on citation, among them:

*"2.6 Authors should represent the work of others accurately in citations and quotations.*

*4.3 Relevant previous work and publications, both by other researchers and the authors' own, should be properly acknowledged and referenced. The primary literature should be cited where possible.*

*4.4 Data, text, figures or ideas originated by other researchers should be properly acknowledged and should not be presented as if they were the authors' own. Original wording taken directly from publications by other researchers should appear in quotation marks with the appropriate citations.*"<sup>[89]</sup>

With time, we think one saw less and less guidance for the budding scientific writer; one's teacher and the literature served. There was an upwelling of interest and writing about citation practice in the years 1963–1979, around the practice of citation indexing pioneered by Eugene Garfield at the beginning of this period. The point was that citation indexing could not be of value unless citation practice was of value. As Gene wrote:



“Obviously citation indexes will be effective only to the extent that the bibliographies in published papers are accurate reflections of the earlier literature.”<sup>[90]</sup>

In his remarkable *Current Contents* columns, which those of us of a certain age remember well, Garfield wrote on numerous occasions, in his wonderful, incisive style, of citation indexing; the fragile individual issues of this small magazine have largely disappeared, but fortunately, Gene's essays have been collected.<sup>[91]</sup> In one of those essays, Garfield also formulated, a succinct list of the reasons why one cites:<sup>[92]</sup>

1. *Paying homage to pioneers*
2. *Giving credit for related work (homage to peers)*
3. *Identifying methodology, equipment, etc.*
4. *Providing background reading*
5. *Correcting one's own work*
6. *Correcting the work of others*
7. *Criticizing previous work*
8. *Substantiating claims*
9. *Alerting to forthcoming work*
10. *Providing leads to poorly disseminated, poorly indexed, or uncited work*
11. *Authenticating data and classes of fact—physical constants, etc.*
12. *Identifying original publications in which an idea or concept was discussed.*
13. *Identifying original publication or other work describing an eponymic concept or term as, e.g., Hodgkin's Disease, Pareto's Law, Friedel–Crafts Reaction, etc.*
14. *Disclaiming work or ideas of others (negative claims)*
15. *Disputing priority claims of others (negative homage)*“

There is substantial overlap with our list.

We owe much to Gene, and this the reason our paper is dedicated to him. Yes, the plague of “impact factors,” and the dubious application of “scientometric” criteria to assign worth to individuals have grown out of his invention. But the abuse of innovations of value is, sadly, human. Eugene Garfield is special. So Harriet Zuckerman writes: “*Gene is extraordinary in so many ways, extraordinary not only for bringing citation indexing into being not just in the sciences but also in the social sciences and humanities but, also, as you know, for making sure the act of citing was placed its very large intellectual context.*”<sup>[24]</sup> And Leah Rea McEwen perceptively says “...*he has always been very open and up front about his techniques and underlying premises. And they are based on core scientific practices such as citation, allowing the individual scholar to knowledgeably participate in the practice.*”<sup>[93]</sup>

Roald Hoffmann has found especially informative a 2004 PhD thesis by Jeppe Nicolaisen,<sup>[94]</sup> which was published in part.<sup>[95]</sup> In Chapter 2 of his thesis, on “Theories of Citing”, Nicolaisen argues that attitudes toward citation are strongly influenced by conflicting philosophical/sociological world views of science. Those with a realist/normative outlook look at citations as one way to communicate faithfully our state of knowledge of the world, gained through experiment and theory. The second group, loosely called social constructivists, view scientific knowledge as socially constructed, and citations then become a tool in that construction. RH, always rooting for the middle,<sup>[96]</sup> sees value in both views, and found

Nicolaisen's tracing of the possible objections out there to Merton's views particularly interesting.

The Nicolaisen article also has an abundant list of references to discussions of citation. We reference a small selection here, with some inclination among the more recent ones for discussions of specific chemical cases.<sup>[97–103]</sup> In limiting here the references we give to a much larger literature, we are painfully aware that we are making the same kind of existential decision that faces every author of a scholarly or scientific contribution.

Also exceptionally valuable is an article by Lutz Bornmann and Hans-Dieter Daniel, brought to our attention by a reviewer. These authors bring together the largest collection of studies of citing behavior that we have seen, and effectively perform a meta-analysis of the literature in the field.<sup>[104]</sup>

As the leading sociologist of science of the age, Merton took a special interest in citation as the currency of reputations. He wrote of standing on the shoulders of giants, as we noted. And he formulated the Matthew Effect,<sup>[105]</sup> and introduced the idea of obliteration by incorporation (he called it the “anatomic or palimpsestic syndrome” in *On the Shoulders of Giants*).<sup>[1,106]</sup> We will end our essay with a Merton citation.

### Modern Times

The case we have shown, and one to come, is an instance of the overt failure of citation practice: the omission of citation of previous work because the work was unknown to the author. Let's give them the benefit of the doubt on that. The failure to cite in these cases is essential to the claims of the paper; the work not cited constituted clear precedent. And even though there was value added in the papers we will mention, it is clear that they would not have been written in the same way had the authors known of the previous work. Would the papers' value have been diminished? Perhaps, although people have unlimited imagination in enhancing the apparent value of their own work. The failure in each case was innocent. And it was also unnecessary; it could have been avoided.

Information technology and the computer have democratized access to the literature. Although it is expensive to subscribe to SciFinder, our anecdotal feeling is that the literature and ways to search it digitally are just more available than before. And not just in rich countries; by hook or by crook, scientists around the world find their way to journals and search tools.

Google, Bing, Yahoo, Google Scholar, and other search engines are just incredible at unearthing information in the scientific literature, even as they visually crowd the webpage with commercial junk. SciFinder, Scopus, and Web of Science are available to most chemists. One has to learn to search. The basic craftsmanship of science searching is largely intuitive, part learned. The advice we will have to give below on this is so self-evident as to seem silly. And yet the obvious was not done, over and over again.

Some searching remains as difficult as it was in the days of a physical library, and the endless shelves, intimidating tomes

of Chemical Abstracts and Zentralblatt in that library. Finding out whether a calculation has been done previously on a CCCF molecule is relatively easy, searching for the products of its dimerization or oligomerization is more difficult. One of us (Roald Hoffmann) was amazed that he could search in SciFinder for a structure with stereochemistry, for example, *trans*-fusions of a cyclobutane with a cyclohexadiene. And amused that some of the hits were not really hits, because someone had to make a decision (an incorrect one) of the stereochemistry of ring fusion in an abstracted paper that failed to indicate precisely that.<sup>[107]</sup>

Somehow, one thinks it should be easier to search for precedent today. And we think it is, showing along the way a new computer-based tool for our specific concern of carbon allotropes. How can it then be that there are such failures of citation? It is as if people's intellectual laziness has grown in proportion to the information technologies available to them!

A perceptive reviewer of this paper objected to our facile blame of laziness. His words are worth quoting:

*“Are scientists today inherently lazier than those of former times or are there other factors—perhaps a multitude if, in fact, the premise regarding failure to cite is sustainable—that need to be considered? Contributing factors might include: i) the movement of recent years towards interdisciplinary research, leading to the requirement of citing literature in a field in which the scientist may not be an expert, ii) the explosion of scientific publications compounded upon the facts taking on a more and more distant significance, resulting in the struggle for the young (and not so young) staying on top of ever-expanding fields as new ones come into being, or iii) the excessive focus on metrics arising from the information age that encourages a culture of rankings trumping the scientific method. In an accelerating culture where time is at a premium and productivity is everything, scholarship stands the risk of suffering in exchange for expediency.”*<sup>[108]</sup>

Well said. We would still argue that there is a computer-age-based incentive to human laziness. We interact with information technology, and see so clearly how efficient computers are at certain things, be it searching on our laptop for a misplaced phrase, or reordering the endnotes in this paper. So when we ask the computer to search for a molecule or a chemical concept, we forget that garbage in is garbage out,<sup>[109]</sup> and in our psychological reliance on what the computer can do, assume that its search—with our limited search phrase—will bring us the world.

So that this paper should not turn into a jeremiad, let us say just a sentence in praise of laziness. In the present context, that human characteristic at least has one good thing about it; it keeps people from including too many citations.

### **Roald's Story: A 3,4-connected net**

Now for the second case of citation amnesia. Again, we beg the reader's forgiveness for the technical detail.

In November 2013, Roald Hoffmann looked at the week's articles in his Old Reader RSS Aggregator, and came upon an interesting paper in the Nov. 19, 2013 issue of Proceedings of the National Academy of Sciences. It was entitled “Stable

three-dimensional metallic carbon with interlocking hexagons”, authored by S. Zhang, Q. Wang, X. Chen, and P. Jena.<sup>[110]</sup> The first Figure in the article looked awfully familiar. It was in fact the unit cell of **tfi**, the structure shown above as **5**, called T6 in the PNAS paper and *glitter* by Roald Hoffmann and Michael Bucknum,<sup>[35]</sup> the latter has published further on this and related nets.<sup>[111–114]</sup> They examined T6 and calculated its electronic structure, its phonons, and its stability. In a smaller part of the paper, another lattice, related to **5**, was examined. Our original paper of 1994 also computed the electronic structure of this hypothetical carbon allotrope, which contains both 3- and 4-connected carbons,<sup>[115]</sup> which are generally called  $sp^2$  and  $sp^3$  carbon atoms.<sup>[116]</sup> It did so with a less sophisticated method than that used in the Zhang et al. paper, but also found it metallic.

The Zhang, Wang, Chen, and Jena paper did not cite our paper. There was absolutely no question of plagiarism; it was clear from the way the work was presented and performed that the Peking University work was original. They just missed our work. Yet our work was not published in an obscure source, but in one of the two top chemical journals in the world! And it was pretty widely cited in the literature to boot.

Clearly we had a bottom-to-top failure of the entire publication process. Neither the four authors, nor the editor for the paper in PNAS (H.-k. Mao; PNAS operates with a system of named editors assigned to a paper), nor the reviewers whose opinion the editor solicited was able to spot a previous paper on the subject in the Journal of the American Chemical Society.

The matter was resolved by my bringing our earlier paper to the attention of the authors, who published a correction. I had to remind one of the authors to also correct a press release that his university had released on the paper.

### **Searching, searching**

What went wrong in the case just discussed? The authors say they searched diligently, yet did not find our paper. It is indeed not easy, and was not in the past (however, it will be easier, as we will indicate below) to search for 3-dimensional networks, or for that matter, for any concept or category. But it's not that hard to do this in the IT age. Here is some self-evident advice for searching:

1. Use several search engines.
2. Think up different ways of getting at the same information, for example, different search terms.
3. Have each researcher on a paper search independently. Perhaps ask someone outside the group to read your paper draft and then search on the basis of an uninformed reading.
4. If you know that a research group has worked in the area, have your junior co-workers go diligently through a publication list of the senior member of that group (usually available online).
5. If you can spot an important early paper in the field, trace references to it through Web of Science.



6. Send an advanced draft to experts in the field, asking specifically if they know of any omitted references.

More generally, we'd advise preemptive training of your students and postdoctoral associates. One variant is to give them another paper of yours, removing the endnotes, and see how many of the essential ones they can reconstruct.

### **How to Deal with Misfortune**

What if, despite diligent searching, you have failed to reference a crucial paper in a published paper of yours? It happens, even to the authors of this unduly preachy paper. In fact, Roald Hoffmann estimates it happens to him in about one third of the too many papers he publishes.

There are two possible circumstances: 1) that you find the omission yourself, after publication, and 2) the author of the missed paper writes to you. Let's take first the toughest scenario, the second one.

In your response to the missed author's letter, **first**, you must not offer excuses, or find fault with the complainer.

**Apologize.** Intellectual property is what scientists treasure, and if that property—ideas, molecules—is not acknowledged by others, it hurts, as we and Bright Wilson and Mario Biagioli said. It just plain hurts. When you have hurt someone, the first thing to do is to comfort or sympathize with them. Just as you would with your son or daughter, if they fell down, no matter whether it was a consequence of some stupid thing they did. Especially you should apologize first if you have caused the pain, even if it was unintentional.

**Second, provide a plan for how you will rectify the fault.** You can say, for instance, "I will be sure to cite your paper in any future publication by me on this subject", or you can offer to put in a corrigendum to your article in the journal.

If instead of these two openings, you begin your response by criticizing the person who complained, as much as you want to do this, and even if it is deserved, then you, and no one else but you, is escalating the emotional level of the discourse. Or to put it in plain English, starting a fight. This is not a good idea; the world has enough strife, between countries, between spouses. Work to defuse conflict, not to create it. No one will think you are a poorer scientist for apologizing. And you will feel better about yourself if you do.

**Third, do not blame your student or collaborators** for the mistake. Maybe they did not do good enough jobs in their literature research, but then 1) for the student, who is it but you who failed to train them to do a good job? 2) for the collaborator, you failed to check their search. In science one trusts everyone, and one is skeptical of everyone, especially of friends, and of yourself as well. Please do not get angry at your wife or husband, or children, just because you messed up.

**Fourth, use the experience to improve** your performance in the future. Think though the first excuses or criticisms of the person whose work you missed that rise to mind. Most such criticisms, such as "The work was published in an obscure (Russian, Chinese, American, open source...) journal", or "The idea was not emphasized sufficiently by the

original authors in their paper" are actually testimony to your laziness, nothing else. Use the fiasco to improve.

Other excuses, along the lines of "Nature (the magazine) lets you have only 30 references; I knew your work, but couldn't get it in", or "My collaborator was the lead on the paper, and he cut the reference out" are transparently only excuses, or evidence of your insufficiencies. If there is a choice of removing a reference of your own versus that of someone else, remove your own. You'll feel better after you do.

Now to the easier case, that when you spot the omission yourself (or someone other than the author of the wronged paper points it out to you). We would recommend the same as above: write to the authors along the first two lines above.

What to do if you spot the omission to cite paper A by paper B, neither your own? Write a polite letter to the corresponding author of paper B, gently pointing out the work in paper A. I wouldn't suggest in that letter that the author of paper B do anything, but people will differ here. Send a copy of your letter to the author of paper A. You will make a friend.<sup>[117]</sup>

We showed earlier two detailed cases of failures of citation practice. We do not just complain, we are intent on doing something about it, even if it is in this quite constrained subfield of solid-state chemistry. The next section shows what we have done; it is inevitably technical and could be skipped by the reader. But he or she should not miss the last Figure, a graphic that epitomizes what can go wrong.

### **A Computer-Age Tool to Help Authors in the Field of Carbon Allotropes**

Honesty in citation practice will never be something that can be delegated to a computer. Ethics is for humans. Davide M. Proserpio and his collaborators Artyom A. Kabanov and Andrey A. Golov have designed a tool that will help future workers in the field of carbon allotropes to avoid duplication and find their way to better citation practice. Had this tool been available to the community, the cases described above could have been avoided.

We searched the literature for carbon allotropes with three databases—Web of Science, Scopus and Scifinder—crossing all the references, extracting the coordinates when available, or asking the authors to provide them, or guessing from the figures and the scant data available in the older references. We examined more than 500 papers (most of them published after 2000) collecting geometrical data (as crystallographic coordinates) for more than 600 allotropes. With the help of the suite of programs for topological crystal chemical analysis ToposPro,<sup>[118]</sup> we compared them in order to find duplicates (often called by different names, as mentioned above), finally extracting 280 unique 3-periodic carbon allotropes. They were of 256 distinct topological types, in other words, different underlying nets: an allotrope containing an inserted C≡C triple bond that just extends the length between nodes 3- or 4-coordinated has the same underlying net as the parent with direct single C–C bonds.<sup>[119]</sup> We assigned a unique name to each, following the same strategy adopted in the analysis of coordination networks. First, if

available, we used the three-letter name in RCSR,<sup>[37]</sup> and then other names already in use for coordination networks. For the remaining 125, we adopted a compact name consisting of a list of the inequivalent 3- and/or 4-coordinated nodes, a capital letter “T” for 3-periodic, and an ordering number. For example, the six allotropes described by Baburin et. al. that were extracted from zeolite nets without 3- or 4-rings<sup>[120]</sup> are named 4<sup>^</sup>6T16, 4<sup>^</sup>6T17, 4<sup>^</sup>6T18, 4<sup>^</sup>7T12, 4<sup>^</sup>8T15, 4<sup>^</sup>8T16, showing that they have 6, 7, or 8 distinct 4-c nodes. The maximal space group symmetry of the nets was found by using *Systre*<sup>[121]</sup> from the *Gavrog* package.<sup>[122]</sup>

All the data are collected and organized as a web table in the Samara Carbon Allotrope Database (SACADA) at <http://sacada.sctms.ru/>. Almost all carbon allotropes are, of course, hypothetical and predicted on the basis of mathematical (topological) reasoning or quantum mechanical calculations, mostly of the DFT type. Different DFT packages have been used to model allotropes and calculate different properties, thereby sometimes leading to results that are not easily comparable.

To help the researcher, we decided to re-compute all collected allotropes using the same level of approximation to extract the relative energy per atom with respect to diamond. All computations were performed using the VASP program suite,<sup>[123]</sup> with an energy cutoff of 400 eV, GGA-PBE pseudopotential; the tolerance for ionic relaxation was set at 10<sup>-6</sup> eV. We allowed full relaxation. The relevant *k*-mesh was generated automatically, as implemented in VASP. The maximal symmetry of optimized structures (output in space group P1) was found by using PLATON.<sup>[124]</sup> Some calculations in the original papers may be better than ours, and still better ones may be performed, of course; the virtue of what we have done is that it is a uniform comparison. Other physical properties were extracted as well and the coordinates of the nets are downloadable for comparison. See the Supporting Information for a listing of the parameters SACADA computes and specifies.

We have learned a great deal in the construction of this database, and would like to share a part of that.

We begin by showing the distribution of coordination numbers in the allotropes in the literature (Figure 1). In Figure 2 we show the distribution of allotropes by computed energy, with the computation performed as described above.

Most of the proposed allotropes are 4-coordinated (Figure 1), while the relative energy plot (Figure 2) shows that all but six have an energy higher than 0.05 eV/C relative to diamond. These six structures are all polytypes or crossed graphene sheets (the networks are shown graphically in Figures S1,S2 in the Supporting Information). The highest energy (3.10 eV), not surprisingly, is for the **nbo** net, where all the nodes have square planar geometry.

The distribution of the reported allotropes with time (Figure 3) shows a renewed interest in the topic from 2011, but also, distressingly, a high rate of repetition. The white areas include some new calculations on older structures. The grey areas are of structures that have been reported in the same year; so they may represent independent discoveries (we have not delved into the relevant submission dates).

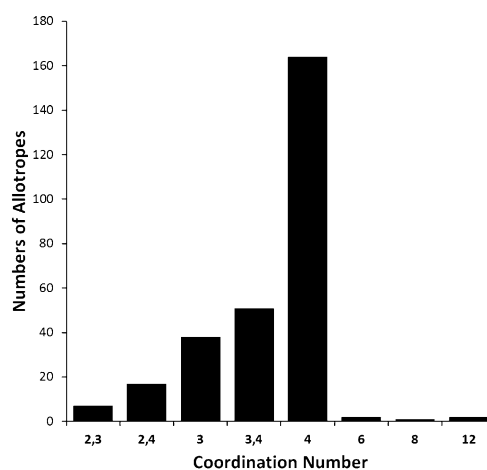


Figure 1. Distribution of allotropes by coordination numbers.

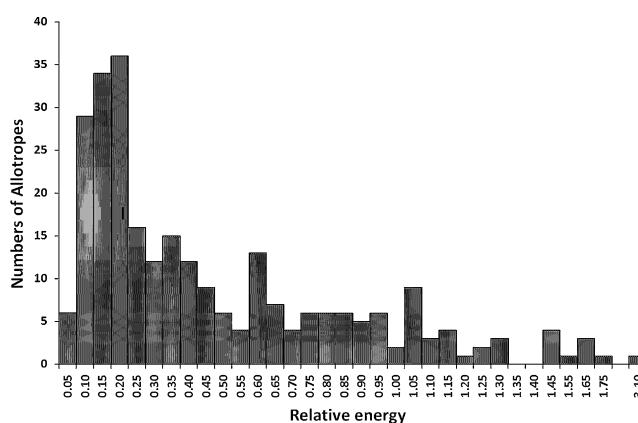


Figure 2. Calculated energies (method described in text) in eV/C atom relative to diamond.

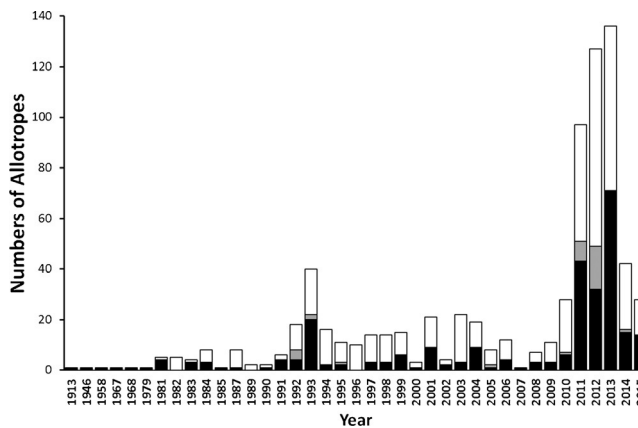


Figure 3. Distribution of new carbon allotropes proposed over the years (in black) and the repetitions (in white). The grey areas are repetitions of structures published in the same year. Note the interrupted time scale before 1989.

The peak around 1991–1995 is due to the stimulus of the suggestion of schwarzites in 1991, named as such in 1992.<sup>[125–127]</sup> Of the 32 new allotropes discovered/computed in that five-year period, there are 14 different schwarzites reported 57 times in the 91 total citations of the same period.

Most papers claim novelty of the structure studied, in one of the many ways that human beings have found of

distinguishing their work from that of others. Sometimes it is not easy to determine if there is a claim. At any rate, there is precious little sign in this dispiriting graphic that greater and easier access to science databases has been utilized by theoreticians in the field.

In the Supporting Information, we provide a searchable spreadsheet (.xls) file with all entries of the database (with full references to 224 articles and all the reported values).

SACADA is an open, living project. We invite scientists to improve it by sending us structures/papers of theirs that we may have missed. Or to use it as they come up with new structures. It will be possible to write to the webmaster of SACADA to check new claims against the nets collected in the database. We plan to additionally include 2D allotropes, since already many claims of “graphene-like” allotropes have appeared in the literature.<sup>[128–130]</sup>

SACADA, as nice as it is (and we are prejudiced), is a tool with a limited range. And carbon allotropes are a small subfield of solid-state chemistry and physics. Perhaps we have been unfair to the available tools for searching of the literature by even choosing this field (carbon allotropes) as an exemplar. SciFinder, CSD, ICSD, and Web of Science all give us wonderful ways to find, for example, a compound of known stoichiometry, a named reaction, the bond lengths of a Eu–Sn bond, or even a chemical structure with stereochemistry. But, as we have said above, it’s much harder to search for an idea or a concept, for example, the anomeric effect, reactions typical of radicals, or fibroid threads with less than 10 nm thickness. That was as true in the days of *Chemical Abstracts* and *Zentralblatt* as it is today.

SACADA is an example of a small database, specific to a specialized subfield of one scientific discipline. It would be easy to build such web-based programs for other subfields, and perhaps as a subfield reaches a critical size, and if there is evidence of people not citing each other as they should, such programs will come into being organically, so to speak. Still, a reviewer of our paper asks: “*in a multidisciplinary field, would a focused approach of compilation akin to SACADA be appropriate or even feasible? Would a transition to smaller, specialized search databases provide better results, or would it introduce more uncertainty as not only do the search criteria need to be effective, but the search medium itself needs to be appropriate?*”<sup>[131]</sup> These are good questions for the future.

We have great confidence in human ingenuity; there are carbon networks waiting to be found. But if you don’t check if a carbon network is already in the literature, you can be sure that diligent editors and reviewers will. Help us get rid of the white sections (see Figure 3)!

### Cite we must, in measure, and with feeling

One could not conceive of science without citations. It’s hard to cite fairly, and in measure. But there is much of value in getting those citations into the paper, often at a late stage of the research, often during the physical act of writing the work up. That may be the first occasion (and we are talking about ourselves) that a cited paper is read carefully, in its entirety. But after all, it’s good that we read them! In contemplating

which citations to include, and which to omit, we negotiate matters of trust and mistrust, priority and influence, history and politics, authority and its denial. It’s done without much thought, far from the considered life. And that’s OK too. For if we do this—write a paper, decide who to cite—repeatedly, we have, willy-nilly, entered the exercise of ethics.<sup>[132]</sup> We need to get there.

We end with quoting Robert K. Merton one more time:

“*The anomalous character of intellectual property in science becoming fully established only by being openly given away (i.e., published) links up with the correlative moral as well as cognitive requirement for scientists to acknowledge their having made use of it. Citations and references thus operate within a jointly cognitive and moral framework. In their cognitive aspect, they are designed to provide the historical lineage of knowledge and to guide readers of new work to sources they may want to check or draw upon for themselves. In their moral aspect, they are designed to repay intellectual debts in the only form in which this can be done; through open acknowledgment of them.*”<sup>[133–135]</sup>

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- [107] Leah Rae Mc Ewen (private communication to R. Hoffmann, Jan. 18, 2016) has pointed out that the human-machine encounter here was not so different from human interactions



- with the old *Chemical Abstracts*, or human–human interactions. What is missing in the present is a dialogue between me (the searcher) and the programmer at *Chemical Abstracts*. We need to work more on this interface.
- [108] Anonymous reviewer of this Essay.
- [109] See Wikipedia article on the first (1963) use of this phrase, and its anticipation by Charles Babbage.
- [110] “Stable three-dimensional metallic carbon with interlocking hexagons”: S. Zhang, Q. Wang, X. Chen, P. Jena, *Proc. Natl. Acad. Sci. USA* **2013**, *110*, 18809–18813; Correction: S. Zhang, Q. Wang, X. Chen, P. Jena, *Proc. Natl. Acad. Sci. USA* **2014**, *111*, 1222.
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- [113] “On the structure of i-carbon”: M. J. Bucknum, C. J. Pickard, I. Stamatina, E. A. Castro, *J. Theor. Comput. Chem.* **2006**, *5*, 175–185.
- [114] “On the n-diamond and i-carbon nanocrystalline forms”: M. J. Bucknum, E. A. Castro, *J. Math. Chem.* **2012**, *50*, 1034–1038.
- [115] The descriptor “connected”, when talking about nets, should be substituted with the more appropriate “coordinated”. Also, “three-dimensional” is better rephrased as “three-periodic” to state the translational symmetry in 3 non-parallel directions: see Ref. [82].
- [116] One of us (RH) prefers not to use the  $sp^2$ ,  $sp^3$  notation because the hybridization in methane (think about how one might measure it!) is not exactly  $sp^3$ , and that in ethylene or benzene not exactly  $sp^2$ . But it’s not something to cross swords on—I understand what people mean when they use the hybridization descriptors.
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- [122] Generation, Analysis and Visualization of Reticular Ornaments using Gavrog <http://gavrog.org/>.
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- [129] The very important initiating paper here, perhaps insufficiently cited, is: “Chemical graphs. VI. Estimation of the relative stability of several planar and tridimensional lattices for elementary carbon”: A. T. Balaban, C. C. Rentia, E. Ciupitu, *Rev. Roum. Chim.* **1968**, *13*, 231–247; Corrigendum: A. T. Balaban, C. C. Rentia, E. Ciupitu, *Rev. Roum. Chim.* **1968**, *13*, 1233.
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- [133] R. K. Merton, Foreword in E. Garfield, *Citation Indexing – Its Theory and Application in Science, Technology, and Humanities*, Wiley, **1979**, p. v–ix.
- [134] Elsewhere, Merton expresses the ideas as follows: “...the bibliographic note, the reference to a source, is not merely a grace note, affixed by way of erudite ornamentation. (That it can be so used, or abused, does not of course negate its core uses.) The reference serves both instrumental and symbolic functions in the transmission and enlargement of knowledge. Instrumentally, it tells us of work we may not have known before, some of which may hold further interest for us; symbolically, it registers in the enduring archives the intellectual property of the acknowledged source by providing a pellet of peer recognition of the knowledge claim, accepted or expressly rejected, that was made in that source.” R. K. Merton, *Isis* **1988**, *79*, 606–623.
- [135] Once you start in this game, it’s hard to stop. Our title phrase, “homo citans” has some currency in the Bulgarian and Slavic literature of literary criticism. See, among others: N. Georgiev, *Tsitirashiat chovek v hudojestvenata literatura*, Sofia, Universitetsko izdatelstvo “Sv. Kliment Ohridski”, **1992**—full text online in the original Bulgarian at <http://litenet.bg/publish/ngeorgiev/cit/content.htm>; N. Georgiev, *Homo citans in Literature*, Sofia, **1980** (this is cited in the preceding reference, but appears to be an earlier thesis by the author, not found); D. Chavdarova, *Homo legens v ruskoj literature XIX veka*, Shumen, Aksnos, **1997**; D. Chavdarova, *Shpon’ka i Oblov-mov—Otsutstvie Chtenia (Otkaz ot Chtenia)*, in Russian, *Russian Literature* **2001**, XLIX, 315–323; D. Czawdarowa, *Homo Legens (Homo citans)—Homo faber*, in *Studia Rossica II: Związki interdyscyplinarne w badaniach rusycystycznych: materiały konferencji naukowej (18–19 listopada 1993 r.)* pod red. Naukow. W. Skrudny, W. Zmarzer.- Warszawa, **1994**, p. 45; “Literature as a factor in man’s spiritual life in the 1830s–1850s (Based on the preface to the Memories of A. A. Grigoriev “My literary and moral wanderings”)” (in Russian), A. N. Larionova, *Philol. Cult.* **2015**, *39*, 186–190.

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