# Enlivening 300 level general education classes on nanoscience and nanotechnology with 3D printed crystallographic models

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## ABSTRACT

Three dimensional (3D) printed models have been utilized in a small sample size study on the comprehension and retention of crystallographic core concepts in a lecture based 300-level general education course at Portland State University. The course's content and goals are described in some detail so that other instructors may gain a better understanding of what we wanted to achieve with both the course and our test of the effectiveness of 3D printed models. Although largely qualitative, the results of this study were overwhelmingly positive. A direct route from open-access crystallographic information framework files to 3D print files and 3D printed models is described and it is hoped that other college educators will design and utilize their own models in their classes. Since 3D printed models can now be designed by individual college educators, it becomes all the more important to tie them as closely as possible to specific course goals. We hope that our work may serve as an example in this respect. The appeal is finally made to other college educators to share 3D print files and supporting teaching material over the Internet.

**Keywords:** *Crystallographic models; 3D printing; materials science and engineering, nano-science and nano-technology*

## 1. Introduction

It has been reported more than a decade ago[1] that more than 150 students who held 3D physical models of molecules in their hands gained a better understanding of their geometric-structural intricacies than they could otherwise obtain from viewing sketches of these models on some two dimensional (2D) support surface alone.

The analysis of data on approximately 400,000 high school students over five decades showed that success in the **s**cience, **t**echnology, **e**ngineering and **m**athematics (i.e. the so called STEM) domains is directly linked to a person's skill in visualizing spatial relations in two and three dimensions[2].

Chemistry and crystallography model kits have for more than two hundred years[3,4] been utilized precisely for the purposes of building up spatial visualization skills and enhancing the students' comprehension and retention of course material in chemistry, mineralogy, crystallography, crystal physics, physical metallurgy, and materials science classes.

As there are also disadvantages to using these model kits (which will be discussed briefly at the end of this paper), 3D printed[5-7] crystallographic models have been brought recently into 300 level general education classes at Portland State University (PSU) with support from the National Science Foundation (NSF) and 3D Systems Corporation. These classes were taught by the first author of this paper as part of a lecture based course under the title: "Introduction to Nanoscience and Nanotechnology". The second author audited these classes out of personal interest.

There are already a few reports on the usage and utility of 3D printed models in college[8-12] education. It was Timothy Herman[12], Arthur Olson[13], and their respective coworkers who started this field more then a decade ago. The Center for BioMolecular Modeling at the Milwaukee School of Engineering (Wisconsin, USA) became under Tim Herman's directorship an instructional materials development laboratory with focus on the molecular biosciences[12]. This center's sister organization, 3D Molecular Designs[14], has a more commercial focus. Arthur Olson, on the other hand, runs both the Science Within Reach LLC company[15] and the Molecular Graphics Laboratory[16] at the Scripps Research Institute in La Jolla, California, USA.

Because we created our 3D crystallographic models[17-19] expressly for the purpose of enlivening classes in the above mentioned course, it is natural that we felt compelled to conduct our own small sample study on the 3D printed crystallographic models' impact on the students' comprehension and retention of selected course material. The results of this study as well as background on the course content and goals are presented in this paper. We are confident that our small sample study on the effectiveness of these kinds of models will soon be complemented by more detailed studies with similar foci but much larger sample sizes.

We consider our paper as topical because there are at least sixteen other groups and individuals that are developing 3D printed chemistry, crystallography, and structural-biology models[9-13,20-31] or use 3D printers in the process of creating such models[32]. As more educators and researchers join this field, the day when any college educator in the world may enliven her or his classrooms with 3D printed models is not far away. This should in principle also apply to Kindergarten through 12 to 14 years of pre-university education, i.e. the so called K-12 and K-14 sectors in the USA. (K-14 includes two years at community colleges.)

In the following section, we describe the course's content and goals in some detail. This is deemed necessary to facilitate a better understanding of what exactly we wanted to achieve with the course, our 3D printed models[17-19], and our test of the effectiveness of these models.

Details on our small sample study follow in the third section of this paper. The fourth section discusses disadvantages of commercial model kits and advantages of self designed models. That section mentions a direct route from openly accessible Crystallographic Information Framework (often referred to by their acronym as CIF) files, file extension *.cif, to 3D print files. Routes to obtain 3D print outs of self-designed crystallographic models are also outlined there.

Our summary and conclusions section contains an appeal to like minded individuals to share teaching material and 3D print files over the Internet. A total of seven short appendices complement the main body of this paper.

## 2. The introductory nanoscience and nanotechnology general education course and its students

### 2.1. Organizational background of the course

The course is formally assigned to the curriculum of the physics department (as that is the affiliation of the instructor), but open to all interested students from the natural and social sciences, all engineering disciplines, as well as all humanities. There are no prerequisites for

this course. The course is not presently part of any major or minor. Consequently, the students in the class elected to take this course, potentially out of personal interest.

The course is part of a sequence of three 300 level general education courses around the wider field of nanotechnology. There is no requirement to take the entire course sequence. Tenured faculty members from other departments teach the other two courses. The titles of those other two courses are "Nanotechnology, Society and Sustainability", and "Nanotechnology: Simulation & Design".

While the first of these two courses is also taught as part of the curriculum of PSU's College of the Liberal Arts and Sciences, the second is taught at PSU's Fariborz Maseeh College of Engineering and Computer Science and is complemented by supporting laboratory work. It is the intention of the instructors of these three courses to support dedicated nanoscience and nanotechnology minors in several departments across the PSU campus in the future.

At PSU, there is also a higher level (advanced undergraduate/graduate) "Introduction to Nano-Materials Science and Engineering"[33] course that builds on these courses. An active community of interdisciplinary college educators that organized themselves into the Portland Nanoscience and Nanotechnology Academy[34] offers supporting nanoscience and nanoengineering laboratory courses.

### 2.2. The course content and goals

We believe that for this general science education course at the 300 level (which requires no prerequisites), an eclectic mix of phenomena at the one to approximately 100 nm length scales and their contemporary technical exploitation needs to be covered in a fairly qualitative manner. After several hours of introductory lectures on the breadth and depth of the field, four main conclusions are reached by the students (guided by the instructor): (*i*) that there is interesting science at the nanometer length scale that goes back some 150 years in its most qualitative form[35] and some 100 years in its more quantitative form[36], but (*ii*) *"there is no such thing as nanotechnology"*[37] just (*iii*) as there is *"no such thing as a nanotechnology industry"*[38,39] and (*iv*) *"no such thing as a homogeneous nanotechnology market"*[40]. This is because nanotechnology is an enabling and supporting technology for many existing industries and markets. Alternatively, it was already clear at the end of the last century that *"there are a variety of nanotechnologies, not just one"*[41].

Some of these statements came as surprises to several of the students in the course. These students may have intended to take the course precisely for the reason of preparing themselves for working in such an industry and participating in such a market. Other students realized that all of this is actually good news and that a strong foundation in the sciences will allow them to be successful in the future.

Nanotechnology is in our course understood and taught as *"the buzzword and an umbrella term to designate nothing less than the state of the art in science and technology in what is the normal progression and evolution of the relationship of humankind with its habitat and environment."*[37] The course goals are best described by the continuation of the previous quote: "*To engage in the nanotechnology discourse is to engage in the science and technology discourse."*[37]

As already mentioned above, a diverse mix of topics from the applied natural sciences (applied physics, chemistry, biology, biochemistry and biophysics), qualifies for such a discourse as it needs to be closely connected to a range of engineering disciplines (electrical, mechanical, chemical, biochemical and biophysical) in order to complement a discussion on contemporary nanometer-length scale technologies.

The natural choice is, therefore, to proceed after the introductory lectures with an introduction to the double discipline materials science and engineering based on a monograph[42] (R. W.

Cahn, *The Coming of Materials Science*) that is very highly regarded in the scientific community. A more recent upper division undergraduate textbook[43] (C. Binns, *Introduction to Nanoscience and Nanotechnology*) and a highly sophisticated popular science book[44] (R. A. L. Jones, *Soft Machines, Nanotechnology and Life*) from which content has been taken for this course break nanotechnology down into *incremental*, *evolutionary,* and *radical* varieties. While the textbook states that "*a lot of incremental nanotechnology"* is in fact only a "*re-branding of other, more traditional lines of research such as materials science and chemistry"*[43], the second book notes that this variety of nanotechnology *"is actually no different in character to what has been studied in fields like metallurgy, materials science and colloidal science for the last fifty years"*[44] (see also appendix A).

What makes nanoscience and nanotechnology different are their foci on the one to approximately 100 nm length scale. Since more traditional materials science and engineering covers all larger length scales, it makes perfect sense to us to consider these new developments as being part of the tradition of *incremental* advancements. Without any doubt, much is to be gained by exploiting the phenomena that are unique to the one to approximately 100 nm length scale. We feel, however, that our students are best served if they gain insights into the wider context of nanoscience and nanotechnology.

Arthur von Hippel's grand 1956 vision about the then emerging field of materials science and engineering, i.e. *"instead of taking prefabricated materials and trying to devise engineering applications consistent with their macroscopic properties, one builds materials from their atoms and molecules for the purpose at hand"*[45], reads indeed much like modern definitions of the *incremental* and *evolutionary* varieties of nanoscience and nanoengineering that are based on nanometer level structuring of custom made materials and devices.

The materials science and engineering (MSE) double discipline has been represented since 1989 by an iconic tetrahedron, the MSE tetrahedron[46]. All four corners of this tetrahedron represent a fundamental core concept[46] of this double discipline. By the tetrahedron's $\bar{4}3m$ point symmetry, all corners of this platonic polyhedron are equivalent so that the four core concepts: (*i*) Structure, (*ii*) Properties, (*iii*) Processing, and (*iv*) Performance are of equal importance when one engages with MSE.

In the case of nano-materials science and engineering, the "nano-core" concepts of Size, Shape, Dimensionality, and Topology[47] need to be covered in addition. Our suggestion is to put all four of these additional core concepts into the center of the MSE tetrahedron, making it the nano-MSE tetrahedron, Fig. 1, which represents the essential content of our course.

Tying the course content to the Nano-Materials Science and Engineering Tetrahedron has the added advantage that no special environmental implications of nanotechnology need to be discussed[33,48]. Note that any remaining concerns about the impact of nanotechnology on society are addressed in the above-mentioned "Nanotechnology, Society and Sustainability" course within our 300 level general education course sequence.

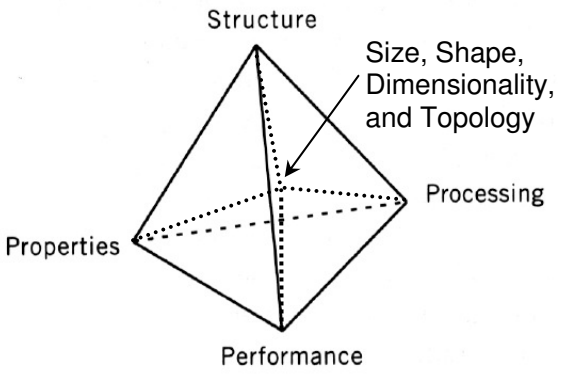


**Figure 1:** The Nano-Materials Science and Engineering Tetrahedron modified after references[33,46].

The practices and opportunities of building materials from their atoms and molecules for the purpose at hand[45] and the *incremental* nanoscience and nanotechnology varieties' preference for the solid state led us directly to utilizing a range of 3D printed models of atomic arrangements in solids and molecules. (This explains why we made crystallography part of the course syllabus. Designing 3D printed models that demonstrate the nano-core concepts of shape, dimensionality and topology to our students are underway.)

*Evolutionary* nanotechnology has been described as the engineering of specific functions into each nano-particle or nanometer structured region of some larger materials entity[43,44]. Integrated electronic circuits and their molecular electronics alternatives are well known representatives of this kind of nanotechnology. In our course, this variety of nanotechnology plays an important role, but a clarifying emphasis is made that success in this field relies entirely on progress in nano-materials science and engineering. (This is actually so since the late 90s of the last century, i.e. since traditional down scaling no longer sufficed and new materials with better properties needed to be developed[49].)

Nanoscience is, accordingly, all about the converging of the traditional scientific disciplines and the energy scales of fundamental processes[50] at the one to approximately 100 nanometer length scale. As there is a full course taught by a senior electrical engineer, i.e. the above mentioned "Nanotechnology: Simulation & Design" in our course sequence, it makes sense to focus the present course on *incremental* nanotechnology (previously mentioned as the "rebranding" of various aspects of materials science, whereby size, shape, dimensionality, and topology are the nano-core concepts) while also covering a few of the basics of *radical* nanoscience.

Since *radical* nanotechnology is all about more or less autonomously acting machines at the nanometer length scale that are constructed out of molecular components[43,44], it is not yet a reality. Our course covers selected topics of the well established scientific foundation of that future field on the basis of the above mentioned books and distinguishes real science clearly from the science fiction and pseudo-science of some well known futurists, see appendix B.

Another main goal of the course is the aiding of the realization in the students' minds of the importance of mathematics in the natural sciences. As atomic-level relations between structures and physical/chemical properties are at the core of materials science, an introduction to basic crystallography is part of our course. This is because (*i*) most technologically important inorganic materials are crystalline, *(ii)* most properties of crystals are anisotropic, (*iii*) crystallography has been generalized[51-55] to the comprehensive science of structures, properties and functions of all forms of condensed matter at the atomic and mesoscopic length scales, and *(iv)* it allows the instructor to introduce simple but very powerful mathematical concepts.

These concepts are the Bravais lattices on which Miller indices are defined and point symmetries that need to be combined with translation symmetries in order to arrive at the space symmetries that crystals can be classified into. Although full mastery of this mathematical framework is not expected from the students, they should ideally gain an appreciation that it is only by abstract mathematics that the atomic structures of crystalline materials becomes comprehensible.

Note that generalized crystallography[51-55], i.e. *"the science of structures at a particular level of organization, being concerned with structures bigger than those represented by simple atoms but smaller than those of, for example, the bacteriophage"*[52], actually forms the "structural foundations" of nanoscience and nanotechnology of all three varieties. Our course only mentions progress in the elucidation and application of non-crystalline and liquid structures[52-55] briefly, but demonstrates structures and functions of physiological important proteins with the help of the interactive Proteopedia web site[56].

### 2.3. Some characteristics of the students in the course

There were 22 students enrolled in this course for credit. Three students opted for the "pass/no pass" grading option. (There were also two senior persons with PhDs in Chemistry auditing on a more or less regular basis.)

As the class was offered both as a general science education course and as a physics course, there was a wide variety of majors of the students. Tables I and II list the study status and declared major for the students that took the class as SCI 382U and PH 382U, respectively.

**Table 1:** Students in the course under the SCI 382U label as a general science education class.

| Study Status | Declared Major |
|---|---|
| Sophomore | Mechanical Engineering |
| Junior | Biology |
| Senior | Social Work |
| Senior | Psychology |
| Senior | Music: Performance |
| Senior | Computer Science |
| Senior | Mechanical Engineering |
| Senior | Science Education |

We inferred from the information provided in these two tables that major differences in the overall course performance are not to be expected simply on the basis of under which course label the students took the course. Indeed later analyses of variance tests performed with the software package Minitab™ supported the hypotheses that there was no statistically significant difference (at the 99 % confidence level) between the midterm and final exam scores of both groups of students.

The average grade of the students that took the course under the label PH 382U was only approximately 4 % higher than the average grade of the students that took the course under the label SCI 382U.

**Table 2:** Students in the course under the PH 382U label as a physics class.

| Study Status | Declared Major |
|---|---|
| Freshman | undeclared |
| Sophomore | Psychology |
| Sophomore | Physics |
| Junior | Physics |
| Junior | Art: Graphic Design |
| Junior | Art: Graphic Design |
| Junior | Mechanical Engineering |
| Senior | Physics |
| Senior | Physics |
| Senior | Philosophy |
| Senior | Philosophy |
| Senior | Business Admin.: Finance |
| Senior | Computer Science |
| Senior | Electrical Engineering |

## 3. The comprehension and retention of crystallographic core concepts study

### 3.1. Goals

The goals of the comprehension and retention study were closely related to the course goals. While it was not expected that the students acquire a comprehensive mastery of selected core concepts of geometrical structural crystallography, they should ideally take away from the corresponding part of the course a deep appreciation that all matter is made up of atoms, that there is an enormous multitude of atomic arrangements, and that the properties of materials are determined by these arrangements.

Our 3D printed models were designed and produced[17-19] primarily to aid this appreciation. The fact that current 3D print/design technologies allow for almost any arbitrary design was very helpful here; any college educator can now come up with her or his own 3D models. We will expand on this in section 4.

The study of the comprehension and retention of crystallographic core concepts was designed

to test the effectiveness of the models for this purpose.

### 3.2. Student recruitment for the study

All 22 "for credit" students in the course were invited to participate in the study in advance, but only 15 showed up for the first part, i.e. special 50 minute long reviews of selected course material with and without the support of 3D printed models. For the second part, i.e. separate testing of identical material during the following lecture period, four more students showed up who were not part of either of these two groups that had a special review of the material at the previous lecture period.

These four students took the comprehension and retention test nevertheless, in effect constituting a second control group. All students in the three groups signed a participation consent form that clarified the goals and procedure of the study.

As most students would probably have preferred to be in the study group (that would have access to the 3D printed models) rather than in the (first) control group (that would not have that benefit), the students were randomly assigned to the study and control group by the course instructor (by literally throwing a die). As mentioned above, a second control group formed from students that did not attend the special course material review on the first day of the study.

The students participated in the study on an entirely voluntary basis. There were no *obvious* incentives to participate in the study other than wanting to learn about the material. It was made clear that (*i*) what is on the comprehension and retention test will ***not*** be part of the final exam and (*ii*) that the results of this test will in no way affect the final grade of any student in the course.

### 3.3. Student group specific preparations for the comprehension and retention test

A set of 17 power point slides that covered the 3D Bravais lattices; cubic and hexagonal densest packings of equal spheres, see Fig. 2; 2D space filling periodic arrangements as combinations of Bravais lattices and motifs (unit cell contents) with certain point symmetries, see Fig. 3; Cu, W, and Mg structural prototypes; halite, fluorite, sphalerite and diamond structural prototypes as derived from the Cu prototype by the filling of interstices; as well as CsCl and $CaTiO_3$ as examples of crystal structures that are based on a primitive cubic lattice, were used in the special preparatory review lectures for the study group and the first control group. These power point slides contained a total of 27 sketches, photos and drawings with an absolute minimum of explanatory words.

One of these sketches and one of the drawings are shown in Figures 2 and 3. Note that 3D printed models of the unit cell of the hexagonal densest packing of equal spheres and the face-centered cubic unit cell that matched what is shown in the bottom row of Fig. 2 were used during the review of the material in the study group.

**Figure 2 needs two columns for proper display and is currently at the end of the paper. This figure needs to show up before Figure 3 as it carries a reference.**

**Figure 3:** Reproduction of a section of a periodic drawing of the artist M. C. Escher[58]. Such drawings are very useful for the demonstration of Bravais lattices, lattice points, unit cells, periodic motifs, and point symmetries within 2D space symmetries.

Both student groups were shown exactly the same set of power point slides, were given (more or less) the same explanations of these slides by the instructor, and in each case the review lectures lasted approximately 50 minutes. Observation notes from both student group review lectures are provided in appendices C.I and C.II. During the special review with the study group, 3D printed models were demonstrated and passed around through the class.

These supporting 3D models comprised unit cells of the hexagonal densest packing of equal spheres, Fig. 4, and unit cells of the simple, body-centered and face-centered cubic Bravais lattices, Fig. 5 There were also opened-up versions of the face-centered cubic unit cell, which exposed the tetrahedral and octahedral interstices in the interior of the unit cell, small spheres that fitted into the interstices and complementary matching pieces to close the unit cell in order to obtain representations of the fluorite and sphalerite structural prototypes, Figure 6. An analogous opened-up version of the unit cell of the hexagonal densest packing of equal spheres was also used, Figure 7.

A "three piece kit" to demonstrate the CsCl structural prototype and its underlying simple cubic Bravais lattice is shown in Figure 8. The above mentioned models were complemented by models of a sucrose molecule and crystal, crystalline sodium chloride, and a $C_{60}$ buckminsterfullerene molecule, Figure 9. All of our 3D printed models have dimensions of several centimeters.

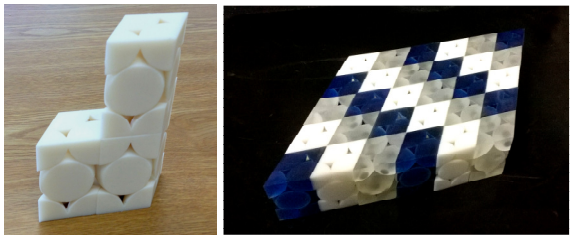

**Figure 4:** 3D printed models of the unit cells of the hexagonal densest packing of equal spheres. The translation and point symmetry, the space and sub-periodic space (i.e. layer) group and their site symmetries can all be demonstrated with a few of these models. (The formation of a hexagonal prism that some students may mistake for the hexagonal unit cell can also be demonstrated.)

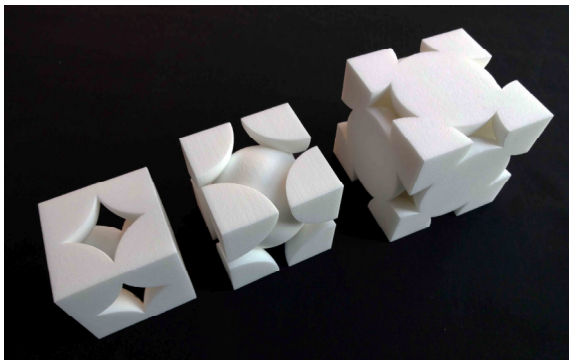

**Figure 5:** 3D Unit cells of the simple, body-centered and face-centered cubic unit cells of equal spheres.

The second control group did not benefit from having the special 50 minutes course material review presented to them with or without the 3D printed models. The members of this group had, however, some prior exposure to about two thirds of this material during the regular course.

The members of the second control group had their test together with the members of the first

control group. During that test, printed out copies of the special review power point slides were available for consultation by the students of both groups, but were mainly consulted by the members of the second control group.

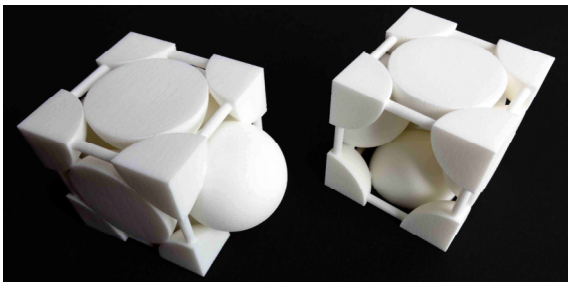

**Figure 6:** 3D printed opened-up version of the face-centered cubic unit cell with exposed tetrahedral and octahedral interstices (right) and complementary matching piece to "close" the unit cell (left).

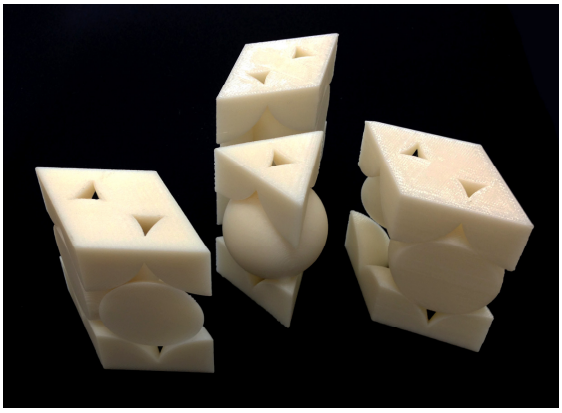

**Figure 7:** 3D printed opened-up versions of the unit cell of the hexagonal densest packing of equal spheres with exposed octahedral interstices and a complementary matching piece to "close" three unit cells.

The members of the study group, on the other hand, had access to both, printed out copies of the special review and the 3D models during their test. Similar to the members of the first control group, the students of the study group did not consult either of these materials much. This is probably because the students of both groups where well aware that the powerpoint slides contained a minimum of explanatory text.

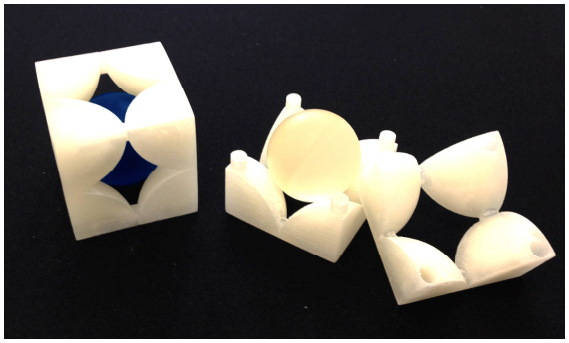

**Figure 8:** 3D printed models to demonstrate the CsCl structural prototype. Left: assembled pieces with a blue sphere in the middle. Middle and right: disassembled pieces and a translucent sphere, representing the $Cs^+$ ion. Without these spheres, the two pieces represent the simple cubic Bravais lattice (i.e. one lattice point per unit cell), see also end of appendix C.I.

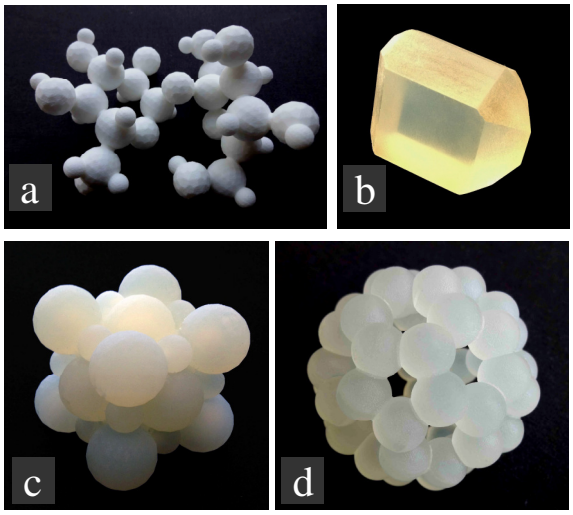


**Figure 9:** Complementing 3D printed models. Top row: (a) sucrose (common sugar) molecule and (b) sucrose crystal. Bottom row: (c) crystalline sodium chloride (table salt) and (d) $C_{60}$ buckminsterfullerene (buckyball) molecule.

### 3.4. The comprehension and retention test itself

**Removed in this version to not bias the tests this quarter**

### 3.5. Test Results and Discussion

The student scores on the comprehension and retention test for the study group (with both special course material review and 3D models), control group I (with special course material review only), and control group II (without review and 3D models) are given in Table 3. The average scores of the test for the study group, first control group and second control group are given in the last row of this table. While the study group and the first control group each had seven members, the second control group comprised only four students. The maximum possible test score was 38 points.

No attempts were made to distinguish between points that had been acquired by comprehension or might be only due to retention or the application of common sense. We believe, however, that some of the points could only be gained by a clear comprehension of the crystallographic core concepts that were tested. This belief is based on the complexity of some of the questions; see for example the caption of Fig. 10.

**Table 3:** Total students' scores by group membership. The final row is the average score for the students listed in the corresponding column.

| Study group | Control group I | Control group II |
|---|---|---|
| 30 | 20 | 12.5 |
| 23 | 17.5 | 11.0 |
| 23 | 15 | 10.5 |
| 19 | 13.5 | 9.0 |
| 16 | 11 | |
| 16 | 10 | |
| 13.5 | 9 | |
| **20.1** | **13.7** | **10.8** |

An analysis of variance test of the data of the first two columns of Table 3 with the Minitab™ software package supports the hypothesis (at the 90 % confidence level) that the study group performed significantly better on the comprehension and retention test than the first control group.

As the sample size of the second control group was approximately 43 % smaller than that of the first control group and the study group, we refrained from further statistical hypothesis testing.

Our qualitative interpretation of the 13.7 and 10.8 point average scores of the first and second control group is that further reviewing of previously covered course material and lecturing on some new material was not very productive when done without the 3D printed models. The differences in the 20.1 and 10.8 point average scores for the study group and second control group, on the other hand, clearly demonstrated to us the effectiveness of the 3D printed models in enhancing the students' learning.

The question remains *why* the students performed so much better than their peers when they had the added benefit of a lecture based review with support by the 3D models. The same kind of question has been asked when students benefitted from virtual reality computer simulations[61], but an answer to such questions may only emerge when the thought processes of the students are investigated and understood.

We leave such investigations to more specialized researchers. Clues to resolving this "mystery" might be found in the history and sociology of science[62].

## 4. Commercial model kits versus self-designed models and direct routes to the latter's design and fabrication

None of the 3D printed models we used in our course are, to our knowledge, part of a commercially available model kit. Models that are built to order may be cost prohibitive as customized designs using traditional subtractive machining technologies require much time for design and execution.

The main disadvantage of commercial model kits is in our opinion, however, that they were designed by *somebody else* and, therefore, not necessarily matched to the intended purpose of the individual instructor. The reason that there are so many different model kits is that they are designed to highlight certain features while unavoidably ignoring and misrepresenting other features[3,62,63].

One may, therefore, need several models that complement each other in order to explain a complex concept comprehensively. 3D printed models have the advantage that one can *design them all by oneself* regardless of their complexity. Prospectively, 3D printed models will be so inexpensive that several of them could be designed by a course instructor to visualize highly complex concepts with this complementarily in mind.

Also 3D printed models are so durable that they can be used in college courses for many years and be exchanged freely with colleagues. Just as an educator needs to tailor information on power point slides from other instructors to her or his own classroom needs, she or he may also feel a need to design 3D printed models for the illustration of complex concepts.

Freely downloadable computer programs[18,64-67] to convert *.cif files[68] into *.stl[69] and *.wrl[70] files that 3D printers understand will come in handy for these designs. (A software license from the University of Washington at Seattle is required only when commercial usages of these programs are intended. While Figure 9a was designed with Cif2VRML[18,62-66], Figure 9b was designed with WinXMorph[18,67].)

While *.stl allows for monochrome printing on all kinds of inexpensive 3D printers and hobbyist machines[4], *.wrl allows for color[71] printing. As mentioned briefly in appendix E, there are already hundreds of thousands of files with extension *.cif in open access and can be downloaded freely from the Internet.

In order to produce 3D printed models, one does not need to "own" a 3D printer. There are commercial (over-night) print shops[72] which will be very happy to do the printing. What one has to provide, however, are the *.stl[69] and *.wrl[70] files of the models.

Also if one is working in a larger college of liberal arts and/or sciences, the institutional workshop or one of the engineering departments will probably have a 3D printer already or get one soon. With the world-wide success of open source self-replicating rapid prototypers, so called RepRaps[5], that can print approximately one half of their own parts, hobbyist 3D printers became economically viable for the average US household[73]. In both cases, one will have to provide the 3D print files in order to produce the models.

In the "working for the greater good spirit" of the forming community of enthusiasts of 3D printing of crystallographic models (see appendix F), we will put our current and future 3D print files with educational relevance for materials science and engineering classes into open access at the PSU Nano-Crystallography Group's website[74].

We will also upload the teaching material of our introductory nanoscience and nanotechnology course (with direct links to the 3D print files of our models) to the National Resource Center for Materials Technology Education (MatEd)[75] at Edmonds Community College in the State of Washington.

Appendix G describes recent efforts by the emerging community of enthusiasts of 3D printing of crystallographic models to create open access 3D print file repositories for both small molecules and macromolecules.

When one has benefitted from the work of others that have put such resources into open access, why should one not share power point slides with supporting 3D print files with other college educators that teach similar classes? Creative commons licenses[76] were created with this kind of application in mind.

## 5. Summary and conclusions

We enlivened a 300 level general education course on nanoscience and nanotechnology with 3D printed crystallographic models. A small sample study on the effectiveness of these models followed.

In qualitative terms, we conclude from this study that reviewing previous course material and lecturing on some new material was of limited effectiveness. Our 3D printed models, on the other hand, proved to be very effective in conveying core crystallographic concepts.

Loosely speaking: while reviewing and more traditional lecturing only enhanced the student's comprehension and retention by approximately one quarter (from 10.8 to 13.7 points on average), reviewing and lecturing with the aid of 3D printed models nearly doubled it (from 10.8 to 20.1 points on average).

Since custom designed 3D crystallographic models can now be produced by relatively inexpensive means by anybody, we look forward to seeing more usage of them in college classes and more studies on the effectiveness of such models.

As for a searchable library of point power slides with supporting 3D print files specific to a range of college courses, let's build it together. The more contributors, the merrier the process will be.

We felt compelled to describe in some detail the course in which the 3D printed models were used. Also we needed to mention the content of the other two courses at Portland State University that complement this course. The breaking down of nanoscience and nanotechnology into incremental, evolutionary, and radical varieties makes perfect sense to us with respect to teaching and studying the subject. Since our course serves also as an introduction to the other two courses, its focus is on both materials science and engineering as well as on phenomena and engineering opportunities at the one to approximately 100 nm length scale (i.e. the incremental nanoscience and nanotechnology varieties).

We felt also compelled to mention that our course deals with some of the scientific basics of the radical varieties of nanoscience and nanotechnology. Discussions of these topics on the basis of well established nanoscience principles should ideally enable the students to make up their own minds on what may eventually become reality and what might remain science fiction and pseudo-science for a very long time (or even forever).

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The other members of the International Advisory Board of the Crystallography Open Database (COD) and the numerous volunteers who helped uploading data are thanked for doing the scientific and science education communities a really great favour.

Ryan Lerud and Andrew Maas of PSU's Nano-Crystallography group are thanked for their work on the educational COD offspring database, the Crystal Morphology Database, and the local COD mirror.

PSU's Human Subjects Research Review Committee determined that the study could go ahead as planned. The head of the Department of Physics determined that the study should go ahead although it slightly reduced the amount of material that can be covered within one quarter.

## References


1. Y.J. Dori and M.J. Barak, *Educ. Technol. Soc.* **4**, 61 (2001).

2. J. Wai, D. Lubinski and C. P. Benbow, *J. Educ. Psych.* **101**, 817 (2009).

3. Q.P. Petersen, *J. Chem. Educ.* **47**, 24 (1970).

4. W.D. Ollis, *Proc. Royal Soc. London* **45**, 1 (1972).

5. A. Bowyer, *3D Printing and Additive Manufacturing* **1**, 4 (2014).

6. B. Berman, *Business Horizons* **55**, 155 (2012).

7. N. Jones, *Nature* **487**, 22 (2012).

8. D. Preece, S.B. Williams, R. Lam and R. Weller, *Anatom. Sci. Edu.* **6**, 216 (2013).

9. H.B. Wedler, S.R. Cohen, R.L. Davis, J.G. Harrison, M.R. Siebert, D. Willenbring, C.S. Hamann, J.T. Shaw and D.J. Tantillo*, J. Chem. Educ.* **89**, 1400 (2012).

10. G.E. Höst, C. Larsson, A. Olson and L.A.E. Tibell, *CBE Life Sci. Educ.* **12**, 471 (2013).

11. V.F. Scalfani and T.P. Vaid, *J. Chem. Educ*. **91**, 1174 (2014); see also B. Halford, *Chemical and Engineering News* **92**, 32 (2014).

12. T. Herman, J. Morris, S. Colton, A. Batiza, M. Patrick, M. Franzen and D.S. Goodsell, *Biochemistry and Molecular Biology Education* **34**, 247 (2006); see also M. Voith*, Chemical and Engineering News* **81**, 36 (2003); *http://www.rcsb.org/pdb/general_information/news_publications/newsletters/2003q2/education_corner.html; http://cbm.msoe.edu/about/publications.html*

13. A.J. Olson, Y.H.E. Hu and E. Keinan, *Proc. Natl. Acad. Sci. (USA)* **104**, 20731 (2007); www.pnas.org/content/suppl/2007/12/05/0709489104.DC1/09489Movie1.mov; see K. Grens, *The Scientist*, July 1, 2012, *http://www.the-scientist.com/?articles.view/articleNo/32285/title/3-D-Printing/, http://models.scripps.edu/*

14. *http://www.3dmoleculardesigns.com/3DMD.htm*

15. *http://sciencewithinreach.com/*, *https://www.youtube.com/watch?v=DB3R6tEHtoA&index=5&list=UULkB0UuveS1NdspqOqQeXGQ*

16. *http://mgl.scripps.edu*

17. P. Moeck, W. Kaminsky and T.J. Snyder, *IUCr Newsletter* **22**, 7 (2014).

18. P. Moeck, J. Stone-Sundberg, T. Snyder and W. Kaminsky, *Proc. Spring 2014 Meeting of the Materials Research Society*, April 21-25, 2014, San Francisco, CA, *in print*, power point slides and audio of this presentation are accessible at MRS OnDemand, (*http://www.mrs.org/on-demand/*), *http://www.prolibraries.com/mrs/?select=session&sessionID=3484*

19. P. Moeck, W. Kaminsky and T. Snyder, *Acta Cryst.* A **70**, C1379 (2014).

20. Y. Watanabe, Y. Ikegami, Y. Murakami, K. Yamazawa and T. Yoshinori, *Acta Cryst*. A**64**, C634 (2008).

21. P. Chakraborty and R.N. Zuckermann, *Proc. Proc. Natl. Acad. Sci. (USA)* **110**, 13368 (2013).

22. T.H. Chen, S. Lee, A.H. Flood and O.Š. Miljanić, *Cryst. Eng. Comm.* **16**, 5488 (2014); see also E. Ratcliffe, *Chemisty World*, April 17, 2014; see also B. Halford, *Chemical and Engineering News* **92**, 32 (2014).

23. P.J. Kitson, A. Macdonell, S. Tsuda, H.Y. Zang, D.-L. Long and L. Cronin, *Crystal Growth & Design* **14**, 2720 (2014); see also E. Ratcliffe, *Chemisty World*, April 17, 2014; see also B.

Halford, *Chemical and Engineering News* **92**, 32 (2014).

24. Y. Teshima, Y. Watanabe, Y. Ikegami, K. Yamazawa, S. Nishio and T. Matsumoto, *Acta Cryst.* A **70**, C1280 (2014).

25. M.L. Hackert and L. Jacquemetton, *Acta Cryst.* A **70**, C1303 (2014); see also *https://docs.google.com/a/pdx.edu/viewer?url=http://www.amercrystalassn.org/app/abstract/download/2181*

*26.* V.F. Scalfani, A.J. Williams, R.M. Hanson, J.E. Bara, A. Day and V. Tkachenko, 248th National Meeting & Exposition of the American Chemical Society (ACS), August 10-14, 2014, San Francisco, CA; *http://abstracts.acs.org/chem/248nm/program/view.php?obj_id=263612&terms*, power point slides of Vincent Scalfani's talk on August 13, 2014 at: *http://www.slideshare.net/AntonyWilliams/accessing-3d-printable-structures-online*

*27.* D. Hurt, NIH 3D Print Exchange, NIH National Library of Medicine, *http://3dprint.nih.gov*, *https://wiki.nci.nih.gov/display/CBIITSpeakers/2014/06/12/July+9:+Darrell+Hurt,+Ph.D.:+The+NIH+3D+Print+Exchange*, see also R. Rettner, CBSNEWS, *http://www.cbsnews.com/news/3d-print-a-brain-with-patterns-from-free-government-library/?utm_source=feedburner&utm_medium=feed&utm_campaign=Feed%3A+tech_talk+%28CBS+News+-+Tech+Talk%29,* June 20, 2014, copyright 2014, *Livescience.com*

28. H. Rzepa, Imperial College London, *http://www.ch.ic.ac.uk/rzepa/*, *http://www.ch.imperial.ac.uk/rzepa/blog/?p=11022*

29. N. Stong, G. Phillips and R. Aranda, University of Wisconsin, Madison, WI; *http://cbe.wisc.edu/assets/docs/pdf/srp-bio/stongrevised.pdf*

30. C. Steffen, Brooklyn, NY, *biologicmodels.com*; see also R. Swaby, *Wired*, August 30, 2011.

31. A. Oakley, University of Wollongong, Australia, *http://www.thingiverse.com/aarono/designs*

32. L. Cuccia, Concordia University, Canada, *http://faculty.concordia.ca/cuccia/contact/*

33. P. Moeck, *Proc. 11th IEEE Conference on Nanotechnology*, August 15-18, 2011, Portland, OR, DOI: 10.1109/NANO.2011.6144299.

*34. http://www.pdx.edu/pnna/*

35. M. Faraday, *Phil. Trans. Royal Soc. London*, **147**, 145 (1857).

36. A. Einstein, *PhD thesis*, ETH Zürich, submitted July 20, 1906, Buchdruckerei K. J. Wyss, Bern; *Annalen der Physik* **19**, 289 (1906).

37. D. Jost, *nccr trade regulations*, Swiss national center of competence in research, working paper no. 2009/21, May 2009.

38. T. Harper, *nanotechweb.org*, May 31, 2002; *http://nanotechweb.org/cws/article/articles/7150*

39. D. Johnson, *IEEE spectrum*, April 25, 2008.

40. E. Toth, *Special Report* 3/30, Autumn-winter (2009), HesaMag #01.

41. I. Malsch, *Nanotechnology* **10**, 1 (1999).

42. R.W. Cahn, *The Coming of Materials Science*, Pergamon, 2001.

43. C. Binns, *Introduction to Nanoscience and Nanotechnology*, Wiley, 2010

44. R.A.L. Jones, *Soft Machines, Nanotechnology and Life*, Oxford University Press, 2004.

45. A.R. von Hippel, *Science* **123**, 315 (1956); *MIT Techn. Rep.* **101**, October 1955; *Molecular Science and Molecular Engineering*, Technology Press of MIT Press and Wiley & Sons, New York, 1959.

46. S.M. Allen and E.L. Thomas, *The Structure of Materials*, Wiley, 1999.

47. S. Gupta and A. Saxena, *MRS Bulletin* **39**, 265 (2014).

48. This is because no captain of industry in her or his right mind will promote and facilitate the development of nano-enabled products in order to deliberately poison or otherwise harm the

potential customers, whose sustained business will be crucial for the long term viability of any company.

49. C.W. Liu, M. Östling and J.B. Hannon, *MRS Bulletin* **39**, 658 (2014).

50. R. Phillips and S.R. Quake, *Physics Today*, May 2006, pp. 38-43.

51. J.D. Bernal and C.H. Carlisle, *Soviet Phys. Crystallogr.* **13**, 811 (1969).

52. A. Mackay, *Izvj. Jugosl. centr. krist. (Zagreb)* **10**, 15 (1975).

53. N.D. Mermin, *Rev. Mod. Phys*., **64**, 3 (1992).

54. A.L. Mackay, *J. Molecular Structure (Theochem)* **336**, 293 (1995).

55. J.L. Finley, *Fundamentals of Physics III – Structure of Solids and Liquids: Crystallography,* Encyclopedia of Life Support Systems, 2009; *http://www.eolss.net/*

56. *http://www.proteopedia.org/wiki/index.php/Main_Page*, J. Prilusky, E. Hodis, D. Canner, W.A. Decatur, K. Oberholser, E. Martz, A. Berchanski, M. Harel and J.L. Sussman, *J. Struct. Biol.* **175**, 244 (2011).

*57. http://practicalmaintenance.net/?p=1051*

*58. http://www.mcescher.com/gallery/*

*59. http://en.wikipedia.org/wiki/Close-packing_of_equal_spheres*

*60. http://en.wikipedia.org/wiki/Sphere_packing*

61. M.T. Springer, *J. Chem. Educ.* **91**, 1162 (2014).

62. M. Charbonneau, *Studies in History and Philosophy of Biological and Biomedical Sciences* **44**, 585 (2013).

63. Limitations of crystallographic ball and stick models are mentioned in the following quote: *"Painted balls connected by rods are less like real atoms than department store mannequins are like real woman."* J. De Ment, *Chem. Eng. News* **45**, 7 (1967).

64. W. Kaminsky, Cif2VRML for windows, *http://cad4.cpac.washington.edu/cif2vrmlhome/cif2vrml.htm*

65. W. Kaminsky, T. Snyder and P. Moeck*, Acta Cryst.* A **70**, C1278 (2014).

66. W. Kaminsky, T. Snyder, J. Stone-Sundberg and P. Moeck, *Powder Diffraction*, Special issue on Crystallographic Software, editor Brian H. Toby, *accepted*

67. W. Kaminsky, WinXMorph for windows, *http://cad4.cpac.washington.edu/WinXMorphHome/WinXMorph.htm*; W. Kaminsky, *J. Appl. Cryst.* **38**, 566 (2005); W. Kaminsky, *J. Appl. Cryst.* **40**, 382 (2007).

68. *http://www.iucr.org/resources/cif* and *International Tables for Crystallography*, Vol. G: *Definition and exchange of crystallographic data*, eds. S. R. Hall and B. McMahon, both in print and on line.

*69. http://en.wikipedia.org/wiki/STL_(file_format)*

*70. http://en.wikipedia.org/wiki/VRML*

*71.* The new Projet 4500 Multijet™ printer of 3D Systems Corporation is currently the only printer that produces 3D color prints in durable VisiJet® C4 Spectrum plastics. Other color printers use the so called "Z Corp technique" and its derivatives, resulting in print-outs consisting of colored gypsum or sandstone based plaster that were dipped into superglue to harden their surface and enhance their stability.

*72. http://www.3dsystems.com/quickparts*, *http://www.shapeways.com/*, and *http://www.sculpteo.com/en/*

*73.* B.T. Wittbrodt, A.G. Glover, J. Laureto, G.C. Anzalone, D. Oppliger, J.L. Irwin and J.M. Pearce, *Mechatronics* **23**, 713 (2013).

74. *http://nanocrystallography.research.pdx.edu*

*75.* The National Resource Center for Materials Technology Education (MatEd) is a NSF funded center housed at Edmonds Community College in the state of Washington; *http://www.materialseducation.org/*

*76. https://creativecommons.org/licenses/*

77. R.W. Cahn, *Nature Materials* **1**, 3 (2002).

78. G.M. Whiteside and A.P. Wong, *MRS Bulletin* **31**, 19 (2006).

79. J.H.E. Cartwright and A.L. Mackay, *Phil. Trans. Royal Soc.* A, **370**, 2807 (2012).

80. K.E. Drexler, *Engines of Creation, The Coming Era of Nanotechnology*, Anchor Books, New York, 1986.

81. K.E. Drexler, *Physics Education* **40**, 339 (2005).

82. N. Taniguchi, *Proc. Int. Conf. Prod. Eng.* Part 2, page 18, 1974.

83. R. Kurzweil, *The Singularity is Near: When Humans Transcend Biology*, Viking Penguin, New York, 2005.

84. L. Osborne, New York Times, December 14, 2003.

85. *http://en.wikipedia.org/wiki/Logistic_function*

86. *http://xkcd.com/1007/*, see also M. L. Green, *MRS Bulletin* **39**, 567 (2014).

87. *http://crystallography.net*; **mirrors** in North America: *http://nanocrystallography.org*, Lithuania: *http://cod.ibt.lt*, France: *http://cod.ensicaen.fr*, and Spain: *http://qiserver.ugr.es/cod*; S. Gražulis, A. Daškevič, A. Merkys, D. Chateigner, L. Lutterotti, M. Quirós, N.R. Serebryanaya, P. Moeck, R.T. Downs and A. Le Bail, *Nucleic Acids Research* **40**, D420 (2012); S. Gražulis, D. Chateigner, R.T. Downs, A.F.T. Yokochi, M. Quirós, L. Lutterotti, E. Manakova, J. Butkus, P. Moeck and A. Le Bail, *J. Appl. Cryst.* **42**, 726 (2009).

88. *http://www.rcsb.org/pdb/home/home.do*; H. Berman, K. Henrick, H. Nakamura and J.L. Markley, *Nucleic Acids Research* **35** (suppl. 1), D301 (2007); H.M. Berman, K. Henrick and H. Nakamura, *Nature Struct. Biol.* **10**, 980 (2003).

89. N. Jones, *Nature* **505**, 602 (2014); *http://www.nature.com/news/crystallography-atomic-secrets-1.14608*

90. *https://listserv.ua.edu/cgi-bin/wa?A0=3DP-XTAL*

91. *http://apps.lib.ua.edu/blogs/3dp-xtal/*

92. list owner's email: *3DP-XTAL-request@LISTSERV.UA.EDU*

93. Royal Society of Chemistry, Crystal Data Repository, *http://api.beta.rsc-us.org/Crystals/v1/cod/* (beta version).

94. *http://www.niaid.nih.gov/news/newsreleases/2014/Pages/3DPrintExchange.aspx*

95. R.M. Hanson, *J. Appl. Cryst.* **43**, 1250 (2010); *http://wiki.jmol.org/index.php/Main_Page*

96. Simplified Molecular-Input Line-Entry System, *http://en.wikipedia.org/wiki/Simplified_molecular-input_line-entry_system*

97. International Chemical Identifier of the International Union of Pure and Applied Chemistry (IUPAC), *http://en.wikipedia.org/wiki/International_Chemical_Identifier*

98. *http://www.micromouse.ca/*

99. *http://www.netfabb.com/download.php*

## Appendices

### A. From metallurgy to interdisciplinary nanoscience

Modern metallurgy grew out of applied chemistry, since the great British metallurgist William Hume-Rothery did his seminal studies on the structures and properties of alloys and intermetallic compounds initially in Oxford University's Chemistry Department. Also materials science emerged "*out of metallurgy by physics*" according to the American industrial scientist Herbert Holomon[77].

Further progress in nanoscience and nanotechnology is to be achieved by bringing molecular and structural biology[78] as well as informatics[79], into the existing interdisciplinary

nanoscience fray that has so far been chiefly defined by chemistry and applied physics.

### B. Science fiction and pseudo-science that is in our course contrasted to the scientific foundations of *radical* nanotechnology

A well known futurist[80,81], who wrongly claims to have coined the term "nanotechnology" (while this was really done by Norio Taniguchi[82] in 1974), and others of his ilk[83] would like the world to believe that perfectly functioning nano-machines, e.g. the ribosome and enzymes, that nature developed over billennia by natural selection on the basis of deoxyribonucleic acid molecules, must be inferior to man-made *assembler*[80] machines (that are either self replicating and may create a *gray goo*[84] or not) simply because they are composed of soft material. By the same argument, that futurist believes that the products of man-made "nano-factories"[81] must be superior to the products of living biological systems.

Our course literally takes pages out of the carefully researched "Anti-Drexler" that Richard Jones[44] authored in order to demonstrate how fantastic the biological nano-machines actually are, precisely because they are dynamical (and soft) systems that evolved to work in salt water solutions at around room temperature where Brownian motion is significant for nanometer sized entities.

Note that an "Anti-Kurzweil" book does not need to be written. This is because the "singularity postulate"[83] of science fiction is essentially debunked by the realization that instead of following exponential functions, all natural growth is much better approximated by logistic functions[85], which do not grow without bounds. The cartoon in figure B1 is in our "Introduction to Nanoscience and Nanotechnology" course utilized to illustrate consequences of allegedly unbound exponential growth.

**Figure B1 needs two columns for proper display and is currently at the end of the paper. This figure needs to show up before Appendix C as it carries a reference.**

### C. Observations and personal impressions of an impartial observer (with a PhD in chemistry) from the 5/15/14 special review lecture sessions

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### E. Crystallographic Information Framework (*.cif) files in open access

As mentioned above, there are hundreds of thousands of files with extension *.cif in open access[87,88] that contain all of the essential structural information of small molecules[87], proteins[88], and small to medium sized unit cell crystals[87]. Utilizing the above mentioned conversion software[18,64-67] (or an alternative conversion route mentioned in appendix F), any college educator can, thus, produce her or his own 3D print files in a straightforward way.

To mention just the two largest open access crystallography databases that allow for free downloads of *.cif files: the Crystallography Open Database[87] (COD) features currently more than 295,000 entries; the Worldwide Protein Databank[88] (wwPDB) features currently more than 100,000 entries. To put these two numbers into perspective, the total number of structures of small molecules, proteins, and inorganic crystals determined each year since 1971 is given in reference[89].

### F. The emerging community of enthusiasts of 3D printing of crystallographic models

A listserv[90] and a wiki[91] site have been set up at the University of Alabama Libraries, where subscribers and visitors can share relevant information. Standing for "3D Printing Crystallography Group", the acronym of these services is 3DP-XTAL. Vincent Scalfani is in charge of this server and the related websites.

Interested readers may contact him per email[92] to join the discussions.

### G. Developments around searchable open access databases of crystallographic 3D print files

Efforts are already under way to create searchable repositories for 3D print files of crystallographic structures[26,27,93,94]. A collaboration between the Science and Engineering Librarian of the University of Alabama Libraries[26] (Vincent Scalfani), the chief developer of Jmol[95] (and JSmol) at St. Olaf College (Robert Hanson), and researchers at the Royal Society of Chemistry (RSC) in the United Kingdom of Great Britain and Northern Ireland (Antony Williams and coworkers) has so far resulted in more than 32,000 *.wrl[70] and 11,700 *.stl[71] files of small molecules[26] that will be made searchable by compound name, chemical formula, SMILES[96], InChI[97], and other characterizers at the RSC's Crystal Data database[93]. These 3D print file entries were derived from *.cif files of the COD[81] with the very popular Jmol[95] program and batch processed to *.stl with the MicroMouse AccuTrans 3D sofware[98]. Whenever necessary, the *.stl files were corrected with the netfabb[99] software.

Based on data of the wwPDB[88], Darrell Hurt and coworkers at the National Institute of Allergy and Infectious Diseases created the National Institutes of Health (NIH) 3D Print Exchange[27]. This database allows users to download, edit and share 3D print files related to health and science[94].

### About the Authors

Peter Moeck (PM) is a materials scientist / applied crystallographer / applied condensed matter physicist with a PhD in crystallography and a thick German accent (about which some students like to complain). He possesses comprehensive postsecondary teacher training credentials from Oxford Brooks College in the United Kingdom of Great Britain and Northern Ireland. He is a (full) Professor of Physics at Portland State University and leader of its Nano-Crystallography Group (http://nanocrystallography.research.pdx.edu/nano-crystallography-group/).

Jennifer Stone-Sundberg is a materials scientist focused on bulk crystal growth and characterization. She completed her Ph.D. at Oregon State University after having taught general chemistry at Portland Community College for several years.

Trevor Snyder received his Master and Ph.D. degree in Mechanical Engineering from Washington State University. Dr. Snyder works for 3D Systems Corporation on the design and development of 3D printers focused on the Multi Jet Printing technology. He enjoys collaboration with individuals on a wide variety of topics including 3D printing applications and metrology, enhanced heat transfer, electronics cooling, materials development, and capillary phenomena. Prior to college, Dr. Snyder spent three years in the United States Army. He has been married for 27 years and has three children.

Werner Kaminsky (WK) is a physicist / chemist / Dr. habilitate of crystallography and Research Associate Professor at the Chemistry Department of the University of Washington with an interest in writing educational software and a talent of attracting requests for providing help on a volunteering basis. He has his own research field around the molecular-structure physical-feature relationship and provides X-ray structure analyses at his department for a living.

PM and WK are members of the International Advisory Board of the Crystallography Open Database.

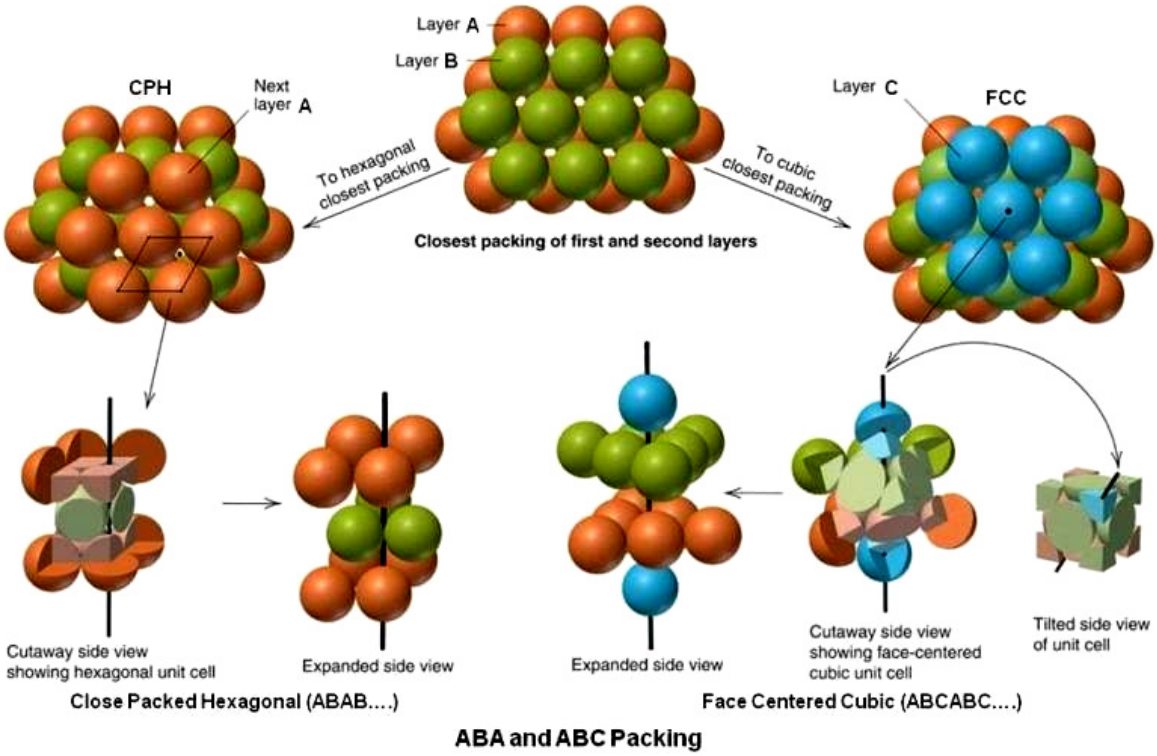


**Figure 2:** Sketch to illustrate the hexagonal and cubic densest packings of equal spheres[1]. Note that the designer of this sketch included "cutaway" representation of the unit cells of the hexagonal (bottom row, left-most figure) and cubic (bottom row, right-most figure) densest packings of equal spheres that are identical to some of our 3D printed models when colors are ignored.

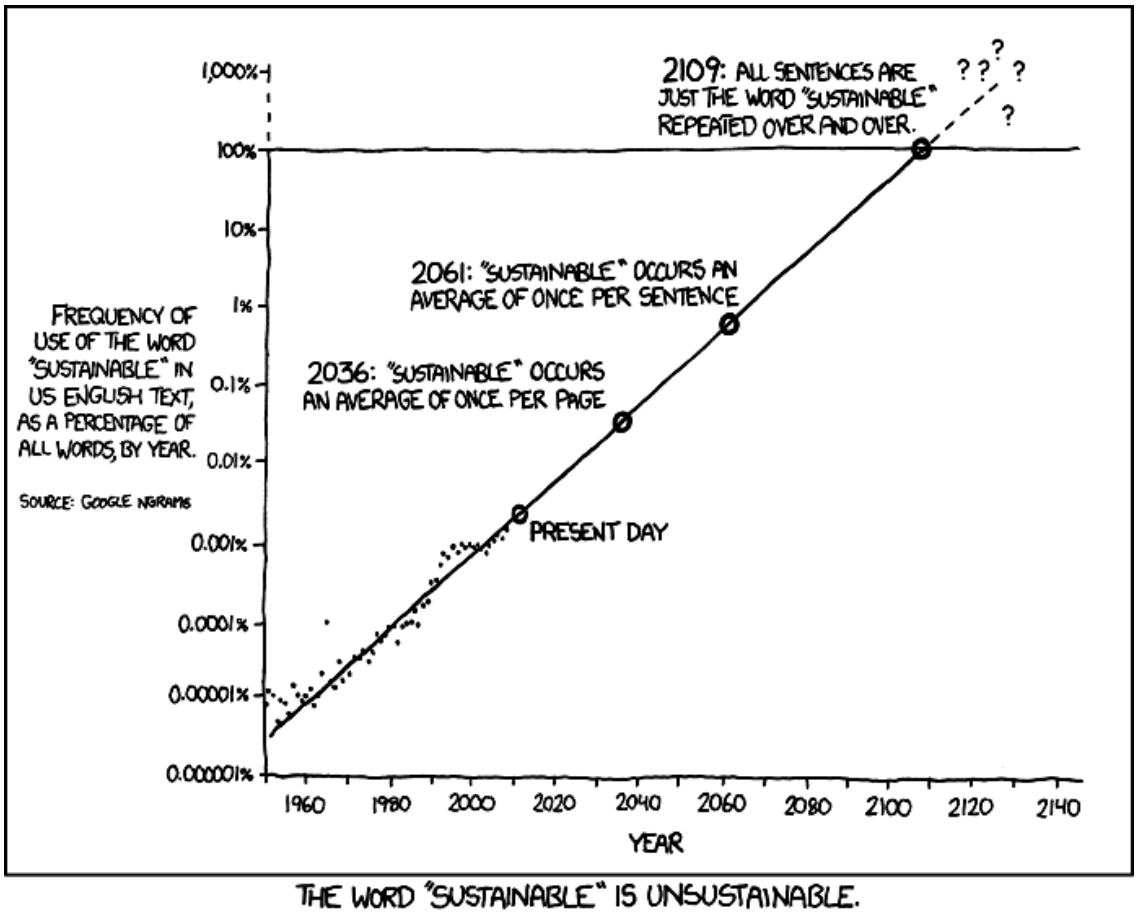


**Figure B1:** The allegedly unbound exponential growth of the frequency of the usage of the word "sustainable" in US English texts over time[86].