



Computational Physics

CrystalNets: A web app for topology determination of crystalline structures

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ABSTRACT

Because topology plays a key role in many chemical and physical properties of materials, identification of topology from crystalline structures is a common and important task in materials science. We present here a new web application, CrystalNets, whose user-friendly interface allows scientists to identify and visualize the topology of crystals from their atomic structure in CIF format. The software has a lot of options to customize its features, such as detection of bonding, choice of clustering model, type of materials (inorganic, hybrid, etc). It has a default mode with powerful heuristics, and allows the user to easily visualize and check the topology detected against the full structure. We also improved the underlying `CrystalNets.jl` Julia library, including a systematic algorithm to handle the complex case of unstable nets.

1. Introduction

The study of the link between the microscopic arrangement of the atoms of materials (i.e., their microscopic structure) and their physical and chemical properties at the macroscopic level is a cornerstone of materials science. The study of structure/property relationships is key to understanding and predicting the behavior of materials, through the laws of statistical physics and the nature of the interactions between the atoms. Going beyond the influence of chemical composition and local geometric characteristics (such as bond distances and angles), features of crystalline materials such as symmetry and topology play a critical role in determining the physical properties of materials [1–3]. The identification of the impact of topology on materials properties has been exploited in a range of fields from condensed matter physics to nanotechnology, [4,5] impacting many physical and chemical properties, such as electrical [6] and optical properties, [7] magnetic properties, [8] thermal [9] and mechanical behaviour, [10,11] among others.

This is particularly true for framework materials, built from well-defined secondary building units (SBUs) linked together by strong interactions into three-dimensional architectures. In such materials, the promise of reticular chemistry [12] is to be able to design periodic solids to attain desired properties and applications by two means: (i) the modification, replacement, expansion and contraction of building blocks; (ii) the control of the topology of the solid (i.e., the net of its framework) [13]. These topology/property relationships have been extensively studied in the topical family of metal–organic frameworks,

subject of a lot of research in the past two decades. Various research groups have detailed the influence of framework topology in MOFs on different chemical and physical properties, [14] including excited states properties, [15] luminescence, [16] magnetism, [17] mechanical behavior, [4] chemisorption, [18] chemical reactivity, [19] gas separation [20,21], guest transport properties, [22] and the emergence of meta-material behavior [23,24].

Therefore, the characterization of materials from their atomistic structure is a relatively common task for materials chemists. Three software have been in wide use for the identification of crystalline topologies: the proprietary ToposPro package for Windows, [25] the closed-source online web tool TopCryst, [26] and the open source Systre software [27]. ToposPro is a reference solution software, offering a lot of options in the processing of crystalline structures, but is closed source and only available on Windows. TopCryst is a fully automated web app, but has very few options in terms of clustering, does not feature visualization of the results, and is also proprietary. Finally, Systre is an open-source code written in Java, but it is not very intuitive to use and does not handle all nets.

To overcome what we saw as limitations of these three packages, we proposed in 2022 a new open-source library for the identification of crystal topologies, named `CrystalNets.jl` [28]. This library was written in Julia, [29] a dynamic programming language that allows implementing complex algorithms with minimal programming effort, while also managing to retain excellent runtime performance thanks to its Just-in-Time compiler design, [30] and which is also easily

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interoperable with other popular languages like Python or C. One of the main goals of this new library was to enable its use at large scale (several thousands of structures) with limited computational cost, for example in the context of high-throughput screening of materials databases.

The `CrystalNets.jl` library has been rapidly adopted by the community and, since its publication, has already seen several large-scale applications. In 2023, Burner et al. introduced the ARC-MOF database of $\approx 280,000$ MOF structures (both experimental and hypothetical), including partial atomic charges derived from DFT calculations [31]. They also added net topology information to their database, through the use of `CrystalNets.jl`. In the same year, Glasby et al. published the DigiMOF database of metal-organic framework structures associated with synthesis information, extracted from publications by text mining, with other 15,000 unique records[32]; they also included topological information through the use of `CrystalNets.jl`. Very recently, topological information was also added to the latest updated of the CoRE MOF database, [33,34] and we published a systematical topological characterization and analysis of more than 150,000 structures of inorganic crystals from the Materials Project database [35].

However, the use of the `CrystalNets.jl` library on one's computer requires programming knowledge, either of Julia, or of Python through the available documented binding. Therefore, we sought to develop a cross-platform, user-friendly interface that would allow non-experts to use the code. Moreover, we wanted to integrate into this a direct visualization of both the input and results, which is very important for manual verification of the results. Encouraged by the widespread use of a previously developed web application in our group (the ELATE [36] software for analysis and visualization of elastic tensors), we developed the `CrystalNets` web app for topology determination of crystalline structures. In this paper, we present its software architecture and design choices, its user interface, and some examples of its use. During the development of the web app, we also worked to improve the underlying `CrystalNets.jl` library since its original publication, and notably overcame the limitation of unstable nets, which we describe in the next section.

2. Improvements to the `CrystalNets.jl` library

2.1. Unstable nets

The topology identification algorithm used by `CrystalNets.jl`, inspired by that of Systre, [27] relies on the computation of the barycentric placement of the net: this consists in placing each vertex of the chemical graph so that it is at the barycenter of its neighbors. Once this operation is done, the resulting position of each node is used to compute the unique topological genome of the structure. However, that latter computation heavily relies on the fact that each placement be unique, in what are termed collision-free nets; or in case of collisions, that adjacent vertices are unique (neighbor-unique nets). Nets that do not meet these criteria are called *unstable* nets. The initial implementation of `CrystalNets` could still identify the topology for a subset of these unstable nets, such that the occurrence of unhandled unstable nets be relatively low:[37] recently the exploration of the entire Materials Project database revealed a number of 152 such unstable 3D nets out of 134,500 (amounting to 0.11%). Yet, the existence of this limitation still prevented `CrystalNets` from being applicable to all possible structures.

The special handling of a subset of unstable nets is now replaced by a general algorithm that can compute the topological genome of any net, unstable or not. Conceptually, the strategy consists in flattening all the vertices that collide in the barycentric placement into a new vertex, computing the genome on this shrunk net, and then lifting it into the genome of the original net. This last operation is done by enumerating all possible permutations among the colliding vertices, computing the resulting genome for each of those orderings, and finally choosing the lexicographically smallest of these genomes.

Two key optimizations allow to reduce the computational cost of the algorithm. The first consists in sorting the colliding vertices by the lexicographical order of their coordination sequence (up to the tenth neighbors): if two colliding vertices have a different coordination sequence, they will be kept in this order through the permutations. Hence, in the extreme case where all the colliding nodes have different coordination sequences, no permutation is required at all. For the second optimization, the genome is compared before and after the permutation of each pair of colliding vertices: if it remains the same for a pair, then the two vertices are equivalent and their respective order will not impact the genome. Such vertices are then grouped together and kept in fixed order. Hence, in the extreme case where all the colliding nodes are equivalent in the previous sense, no permutation is required again.

In order to identify a topology, a preliminary step requires to minimize the net, that is, finding the smallest unit cell corresponding to the periodic graph. The original strategy consisted of listing the possible translations that could map a vertex of the graph to another, then checking whether the translation was valid for all the other vertices and edges. However, this latter check is not straightforward in the presence of collisions. For this purpose, we implemented a backtracking algorithm that attempts to perform such a mapping, and also uses the coordination sequences of the colliding vertices as an optimization.

Due to the enumeration of permutations, the complexity of the entire algorithm grows from being polynomial in the size of the net [27] to factorial in the maximum number of vertices that collide in the barycentric placement. However, runtime performance remains completely unaffected for stable nets and does not noticeably evolve for the previously handled unstable nets. Only rare unstable nets may thus require up to significantly more time than the others. This situation can exceptionally result in the web interface failing to return the topology within the time frame of one minute, after which a timeout occurs to make the server accessible again: in this case, the user is invited to use the Julia library instead to run the computation to the end. Overall, `CrystalNets.jl` can now identify the topology of all nets.

2.2. Hydrogen bonding

The topology of a material is an abstraction built on the structure of the network of its chemical bonds. In that regard, some materials exhibit particular topologies only when considering special kinds of bond, and options for tuning the selection of bonds have been available to the user from the start. An important new addition to them is the possibility to automatically detect hydrogen bonds, of particular interest in the topological analysis of structures such as clathrate hydrates.

In addition to the standard heuristics for bond detection, which relies on the van der Waals radius of the two atoms and their distance, the specific case of hydrogen bonding requires identifying three atoms: the hydrogen H, its electron-rich covalent neighbor D, and the lone-pair bearing H-bond acceptor A. For simplicity, we restrict the latter two atoms to the elements O, N, F, Cl and S. Then, for all pairs of an acceptor A and a bonded D–H, we compute the A...H distance and the D–H...A angle. Only the pairs that have a distance lower than 2.5 Å and an angle higher than 150° are deemed acceptable, and among them, the pair with the smallest A...H distance is kept. The maximum distance, angle, and number of pairs kept are options that the user can adjust.

2.3. Miscellaneous

The `CrystalNets.jl` library now includes a few more features that may be helpful in particular situations:

- It is possible that multiple substructures occur in the same unit cell, each with their own net — in particular in the case of interpenetration, which is frequent in metal-organic frameworks[39] as illustrated in Fig. 1. For detailed reviews of interpenetration in periodic networks, we refer the reader to Refs. [40–42] and [43]. The latest

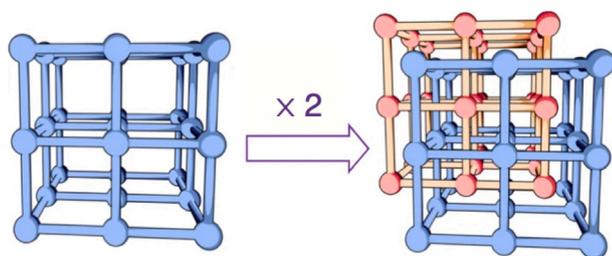


Fig. 1. Illustration of a simple two-fold interpenetration in the 3D MOF β -MUF-9, where each net corresponds to a simple cubic lattice[38]. Adapted with permission from Ref. [38]. Copyright 2023 Springer Nature.

version of `CrystalNets.jl` provides the full list of periodic substructures identified, their topology (in the case of Fig. 1, *pcu* or “simple cubic”), and allows to selectively display them in the viewer.

- A common source of bonding errors came from the presence of carbon cycle disorder in the input files obtained experimentally on MOFs. The cleaning heuristics of `CrystalNets.jl` are now capable of recognizing this in many cases, as well as a few more sources of disorder, and correctly assessing the bonds in their presence.
- A previous heuristic used to systematically split vertices that consisted of a single oxygen into edges that bond their neighbors. This option is now disabled by default to more accurately compute the topology of inorganic materials, but remains set by default for MOFs and zeolites.
- For the library users, it is now possible to track the mapping of the vertices from the input to the topological genome.
- A Python tutorial is now available in the documentation to streamline the use of `CrystalNets.jl` from a Python coding environment.

3. Architecture of the web application

3.1. Web applications: Server or client-side?

The choice of a web application for `CrystalNets` was an easy one: contrary to desktop applications, web apps run in any user’s browser, on a variety of platforms (computers, tablets and even phones), and without requiring the need for installation. Moreover, the combination of modern HTML and JavaScript standards allows for the easy design of user interfaces in a cross-platform language. Our previous experience with our ELATE tool [36] had shown us that this low barrier of use for other scientists makes the web app very appealing, translating into very large usage. At the time of writing, ELATE is used about 4400 times per month, and the corresponding paper has about 1500 citations, which we consider a large success for a relatively niche use case.

When designing a web application for scientific calculations, the most important question is to decide whether the core of the numerical work will be performed on the server side or on the client side. In the first case, the user’s browser (the “client”, in network terms) is only used as an interface, requesting and displaying data from the web server: all the calculations are performed on the server. Among the upsides of this choice: we control finely the software stack on the server, so we can run any type of code, and it can be more powerful (and therefore faster) than running code inside the user’s browser. There is one downside, even if the computation does not take a lot of time: this model is hardly scalable, and if there are a lot of users, the server will not be able to answer all requests.

For the second option, in the case of client-side calculations, the browser itself will be running the calculations. This is interesting because it does not require a powerful server, but it does add strong constraints. First, browser-side execution is limited to short tasks (a few seconds at most), because the browser will otherwise “freeze” and stop the CPU-intensive task. Secondly, this requires the computation to be

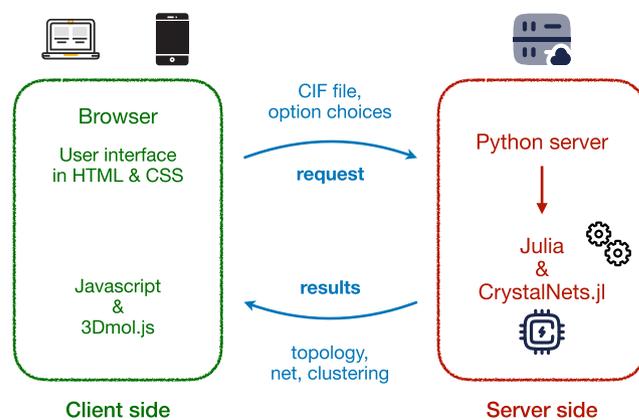


Fig. 2. Schematic architecture of the `CrystalNets` web application, with computations performed by the Julia code on the server side.

written in (or compiled into) either JavaScript or WebAssembly code, which all modern browsers can run. While options for compilation of various languages into WebAssembly are expanding (it is now possible for C and C++, and Python support is experimental), this is not currently possible for Julia on such a complex library as `CrystalNets.jl`, so it was not an option for `CrystalNets` at this time.

3.2. Software stack

Therefore, we wrote `CrystalNets` as a server-side web app, whose architecture is schematized in Fig. 2. The user interface is written in HTML and CSS, displayed in the browser, and when the user chooses a CIF file for analysis, that CIF file and the list of options chosen are transferred to the server in a HTTPS POST request. The server uses the Flask Python framework to serve web pages, and calls Julia with the `CrystalNets.jl` library to run the topology identification. Because of the Just-in-Time compilation model used, Julia programs can be very fast to run but relatively slow to start: this issue is particularly visible in the context of a web service, so we circumvent it by using the `DaemonMode.jl` Julia library to keep the Julia backend reactive. The results usually take around a second to be computed, and are then returned to the browser where the JavaScript-based `3Dmol.js` interactive viewer[44] is used to display 3D models of the input structure, nets and clustering information.

The web application is hosted on a virtual machine accessible at <https://progs.coudert.name/>, which also hosts other online tools produced by our group.

4. Interface and features

4.1. Overview of the interface

Fig. 3 displays a screenshot of the interface of the `CrystalNets` web app, after the topology identification of a crystal structure (in this case, a hydrated model of the HKUST-1 metal–organic framework). You can see it is divided between the following areas:

- Top-left: the results of the topological analysis. In this case, for the two main choices of clustering, the net is identified as **tbo**.
- Below that: some information messages and warnings. Here, `CrystalNets` was provided a structure without bonding information, so it used heuristics to detected bonds. Also, it identified unconnected molecules (the water) that were ignored for topology calculation.
- Further below: an upload box, where you can upload another structure to run `CrystalNets` again. You can also modify the options that were used (structure type, choice of bond detection, choice of clustering methods).

Results for HKUST-1-with-water.cif:
AllNodes, SingleNodes: [tbo](#)

CrystalNets emitted some warnings:
Warning: Guessing bonds with custom algorithm (from Chemfiles and VMD). This may take a while for big structures and may be inexact.
Info: To avoid guessing bonds, use a file format that contains the bonds.
Warning: Detected 48 structures of dimension 0 in HKUST-1-with-water, possibly complex solvent residues. They will be ignored for topology computation.

Upload a CIF file, or any other crystallographic file format accepted by [chemfiles](#), here:

No file selected

Submit

Main options:
 Structure type: [?]
 Auto MOF Cluster Zeolite Guess
 Bonding: [?]
 Auto Guess Input H-bonds
 Clusterings: [?]
 Auto SingleNodes AllNodes Standard PE PE&M Input EachVertex
 Exports: [?] (check [the tutorial for visualization](#))
 Input Trimmed Subnets Attribution Clusters

3D visualization of the topology identified, overlaid on the input structure. The visualization is customizable, through the clickable buttons just below:

Home | Input | Trimmed | Clustering | X
 AllNodes | SingleNodes

Fig. 3. Screen capture of the results of the CrystalNets web app for a structure of hydrated HKUST-1 metal–organic framework.

- Right side: interactive 3D visualization of the topology identified, overlaid on the input structure. This visualization is customizable, through the clickable buttons just below.
- At the bottom, you can export the results of the calculations: in particular, you can download the subnets and clusters as VTF files (readable by molecular visualization software like VMD [45]).

Regarding the input files, CrystalNets deals primarily with files in CIF (Crystallographic Information File) format, which are the gold standard for the representation of crystal structures [46]. The CIF file format allows for a complete representation of the crystal unit cell and content, including space group and symmetry elements, and can optionally contain information about chemical bonds (i.e., which atoms are considered bonded in the structure). Although we recommend the use of CIF files as input, CrystalNets can also read other formats representing periodic systems, such as PDB files, through internal use of the Chemfiles library which supports a large number of different formats [47].

4.2. Options for topology determination

We aimed to make the web app easy to use even for scientists not familiar with details in the topology of crystalline structures. Therefore, the main choices are clearly delineated, and have reasonable default settings and short explanations. The first important choice is the specification of the **structure type** for the crystal: this choice impacts the bond detection algorithm as well as the clustering used, allowing for example to fine-tune the algorithm parameters for specific materials families, such as MOFs or zeolites.

The second set of options controls the detection of **bonding**: the topology is based on the molecular graph, and crucially depends on the definition of which atoms are bonded to one another. If the input file format (typically a CIF file) specifies the bonds, they will be used by default. However, when they are absent, or if they are deemed too unusual, CrystalNets will use its own heuristics to detect bonding patterns – it can be tuned for specific structures (see above) and can include hydrogen bonds or not, depending on user choice. An explicit bonding choice other than the default ensures that either the input bonds are used, if the bonding heuristics are invalid, or to force CrystalNets to guess the bonds if those stored in the file are inadequate.

The third important option is the choice of **clustering** of atoms into secondary building units, answering the question: how do we decompose the atomic structure into a net? The simplest choice is to give each atom its own vertex (the EachVertex option), and simplify the net from there: vertices with degree 2 or lower are iteratively collapsed into edges until all vertices have degree 3 or more. This is well adapted for dense inorganic structures, but not suitable for supramolecular frameworks. For more complex structures, such as metal–organic frameworks, we have implemented four different options proposed in the literature: “all nodes”, “single nodes”, “points of extension” (PE) and “points of extension and metals” (PEM), whose conceptual differences are summarized in Fig. 4. Additional clustering options are also provided for these specific cases:

- the standard clustering as performed in the ToposPro software[25, 26] corresponds to the Standard option in CrystalNets;
- user-defined clustering (the Input option), provided in the input file;
- Auto for automatic determination based on structure type.

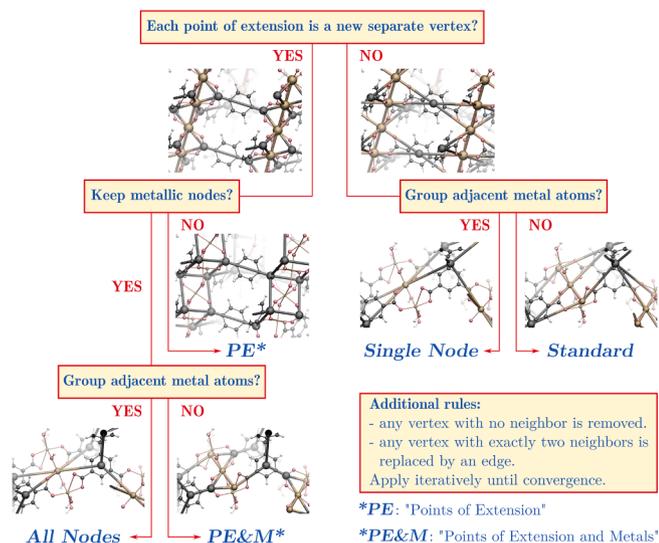


Fig. 4. Schematic decision tree for the different choices of clustering. The top and middle-left panels are illustrated on the case of MIL-53 framework[48]. The bottom-left and middle-right panels are illustrated on the CSD framework ALIXUP [49].

Additional options:
See detailed help in the [manual of CrystalNets.jl](#)

Ignore atoms (comma-separated list of atomic types):

Ignore homoatomic bonds (comma-separated list of atomic types):

Cutoff coefficient (floating-point number):

Maximum polyhedron radius (positive integer):

Maximum H-bond distance, if H-bonds option is set (floating-point number):

Maximum H-bond angle, if H-bonds option is set (floating-point number):

Maximum number of H-bond per H, if H-bonds option is set (positive integer):

Bond adjacent SBUs

Authorize pruning

Wider bonds for metals

Ignore homometallic bonds

Reduce homometallic bonds

Ignore metal-cluster bonds

Ignore low occupancy

Detect paddlewheels

Detect organic cycles

Detect points-of-extensions

Cluster simple points-of-extensions

Separate metals

Pre-merge metal bonds

Split lone O vertex

Unify SBU decomposition

Use atom label instead of type

Skip minimize

Ignore types

Fig. 5. List of additional options (advanced settings) offered by the CrystalNets web app for power users. Full description of each setting is provided in the online documentation at <https://coudertlab.github.io/CrystalNets.jl/dev/lib/public/>.

We refer the interested reader to Ref. [28] for a full description of each specific algorithm, or to the online documentation at <https://coudertlab.github.io/CrystalNets.jl/dev/lib/public/#CrystalNets.Clustering>

Finally, we note that more advanced methodological choices are also available for power users, beyond these three main options. We list in Fig. 5 the full list of advanced options available from the web app, which corresponds to the options of the underlying `CrystalNets.jl` library — and are linked to the library documentation for reference.

4.3. The naming of nets

Once CrystalNets has decomposed the crystal structure into one or more nets, it determines the topology of the net through a unique identifier called the *topological genome*: a series of numbers (e.g., 3 1 1 0 0 1 1 1 0 1 0 1 1 1 0 0) that uniquely defines the net, regardless of any permutation of edges or other transformation. This is useful for classifying nets and making statistics, but not very readable. Therefore, CrystalNets also compares the net with genomes of known nets from existing databases, to identify if the net has been reported before. CrystalNets relies on three different databases: the Reticular Chemistry Structure Resource (RCSR) database,[12] the EPINET project,[50] and the Structure Commission of the International Zeolite Association (IZA-SC) database[51] for zeolites. If the net is identified, then CrystalNets will refer to it through its common name: for example, the net with 3 1 1 0 0 1 1 1 0 1 0 1 1 1 0 0 as genome corresponds to primitive cubic lattice, denoted by the **pcu** code in the RCSR database, and can be visualized online at <http://rcsr.net/nets/pcu>.

In many cases, CrystalNets will identify the net (or nets) of the crystal structures, but they are not listed in any of the databases. In such cases, the result displays a custom 14-character name consisting of the dimensionality of the net, a hyphen, then 12 letters obtained by hashing the topological genome through SHA-224. It is important to note that the databases only contain a fraction of the topologies encountered when studying materials science, and thus a result with such a custom name is a common occurrence. Indeed, a recent systematic survey of the Materials Project database of inorganic materials highlighted the very large diversity of topologies: the analysis identified 38 430 different topologies, but only 719 of these nets were present in any of the topology databases (amounting to 1.9% of topologies)[35]. Combining these 38 430 topologies with the ones from a theoretical zeolite database [52] and the known topologies from the RCSR, IZA-SC and EPINET, we obtain more than 700 000 different unique nets: although name collisions could theoretically occur in the computation of the custom 14-character name, we checked on this large dataset that the identifier computed in this fashion was always unique.

4.4. Limitations of the topology determination

In this section, we want to highlight some of the caveats and limitations of the methodology for topology determination, in general and in the CrystalNets web app. Most of these limitations are linked to the choices of methodology, rather than its specific implementation, but they are important enough for users that we want to highlight them here. The first is the necessary reliance on the presence of accurate bonding information: this means that users should either provide input CIF files with bonds present (using the `geom_bond_*` CIF items)¹, or double-check the result of the bond detection heuristics employed by the software (which can be done in the visualization window of the app).

A second caveat is the fact that topology identification is challenging in the presence of disorder in the crystalline structure. In practice, disorder may be the most common reason when a topology was not recognised or not recognised correctly, when applied to experimentally-determined structures without any cleaning up [53]. While `CrystalNets.jl` has been updated over the past two years with improvement to its heuristics for the detection and handling of certain types of disorder, there is no generic solution and users must carefully check the net decomposition visually. We note, however, that on a test set of experimental MOF structures, the heuristics in `CrystalNets.jl` were sufficient to handle disorder without human intervention in 80 out of 100 cases [53].

¹ Core dictionary (coreCIF) version 2.4.5, Category GEOM_BOND, available online at https://www.iucr.org/_data/iucr/cifdic_html/1/cif_core.dic/Cgeom_bond.html

5. Conclusions & perspectives

We have described here the CrystalNets web application, which we have developed and are hosting for materials scientists to analyze the topology of their crystalline structures. Based on a core library in the Julia language, the web app allows for a user-friendly interface and choice of documented settings for materials scientists who are interested in the topology determination of crystalline structures, without having in-depth experience. It also means that there is no requirement for local installation of the software, and it can run on any computer, tablet or even phone. We believe that offering scientific tools for analysis and visualization as web apps is an appealing venue for both users and developers. Made possible by the advances in modern web standards (HTML, JavaScript, WebAssembly, WebGL, WebRTC, etc.) and browser support of these standards, it allows for cross-platform development with relatively low overhead. We think it is particular well-suited for small computations that run in under ten seconds, and encourage other scientists to develop such tools for the community of materials scientists.

CRedit authorship contribution statement

Lionel Zoubritzky: Writing – review & editing, Writing – original draft, Software, Methodology, Investigation, Conceptualization; **François-Xavier Coudert:** Writing – review & editing, Writing – original draft, Supervision, Software, Methodology, Investigation, Conceptualization.

Data Availability

No data was used for the research described in the article.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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