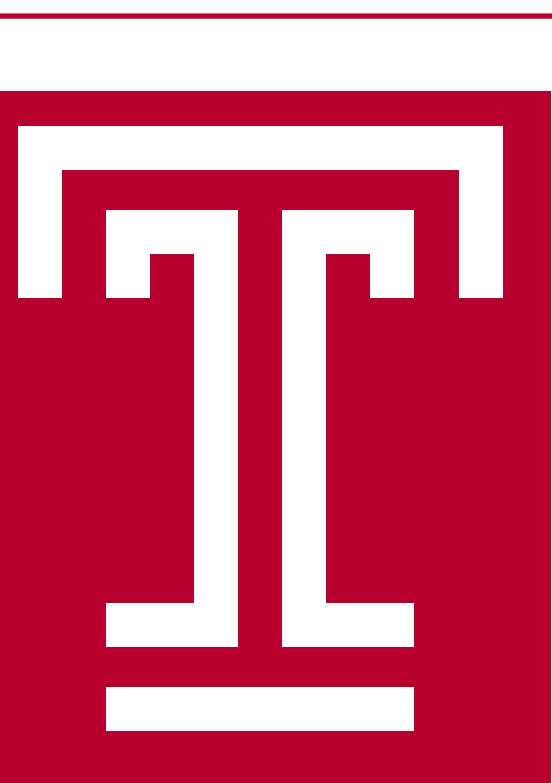


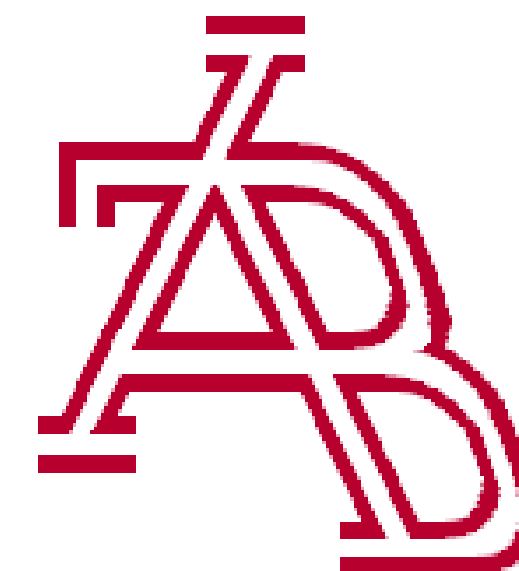


# DECOR: The Database of Educational Crystallographic Online Resources, Updates and Prospectus

DECOR site: <https://decor.cst.temple.edu/> (or google: “DECOR crystallography”)

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## Abstract

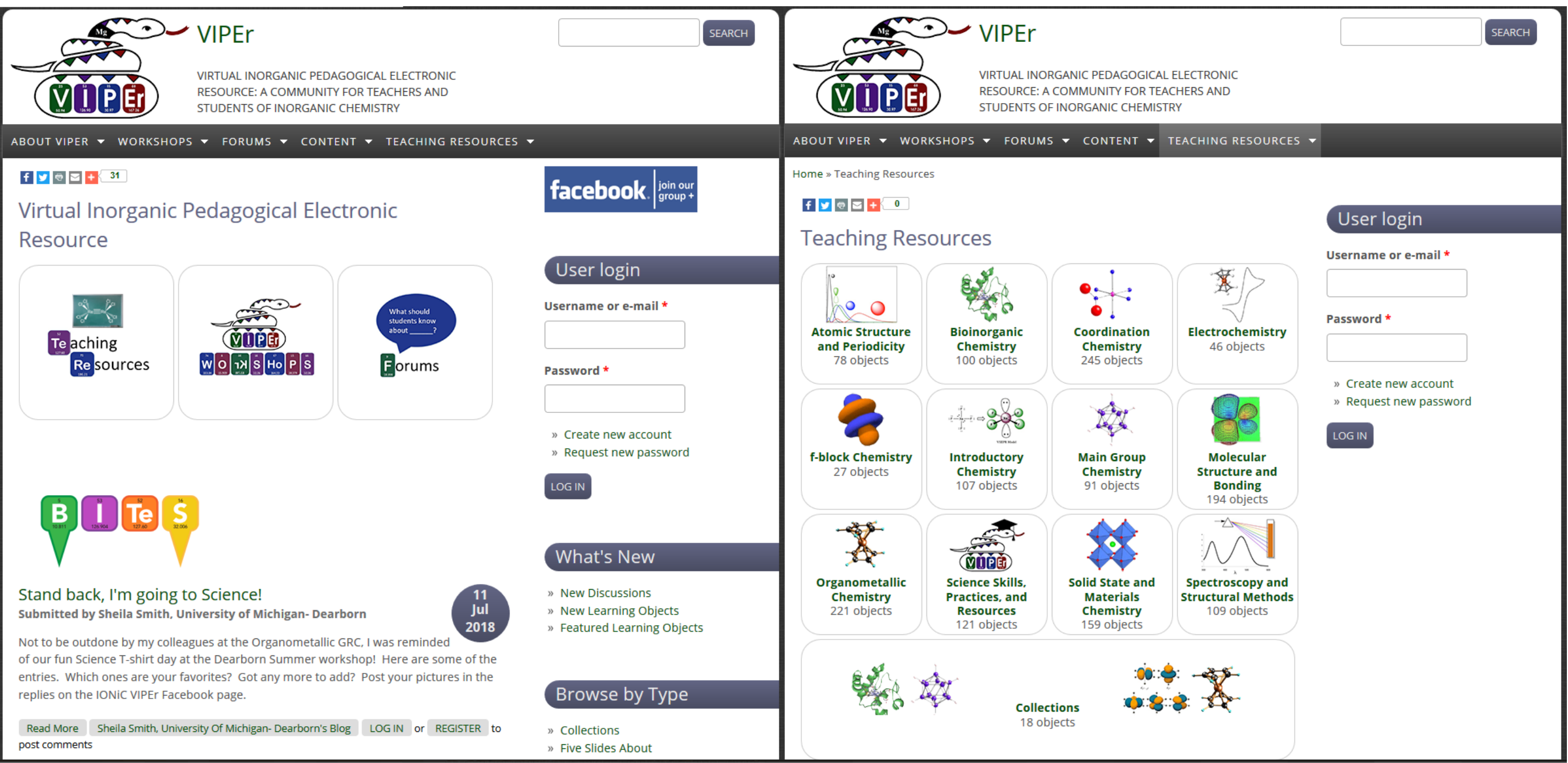
The Database of Educational Crystallographic Online Resources (DECOR) is the worlds first repository for educational resources for the teaching of crystallography and diffraction. The site, available at [decor.cst.temple.edu](https://decor.cst.temple.edu/), permits the sharing and downloading of educational resources such as practice problems, visual aids, animations, and more. The site is currently organized into three basic resource layouts: 1) Resources by Type, where visitors can browse for homework problems, presentations slides, or animations across topics. 2) Resources by Topic, where visitors can look for resources relating to particular subject matter such as the reciprocal lattice, scattering, or symmetry. 3) Links, which sends visitors to other sites that provide convenient resources for crystallographic education. The purpose of the poster is to make attendees aware of this teaching resource, and to present the current state of the site, and plans to upgrade and enhance it in the near future.

## Inspiration

In 2009 when I began my academic appointment at Temple University, I proposed to modify an existing course entitled “solid state analysis” which had been taught by the late Prof. Donald Titus, who taught it as a survey course of techniques to examine the solid state, with X-ray crystallography being a small part. In my own crystallographic education under Doug Ho and Sonny Lee at Princeton, I first learned the operation of the instrument and software with minimal understanding of the underlying physical concepts. Later, as a postdoctoral worker at Purdue, I audited a course in crystallography taught by Phil Fanwick, which was mostly theoretical in nature, but filled in some of the gaps in my theoretical learning. Since that course, I have had an interest in developing a course that takes a holistic approach to crystallographic education, combining theoretical learning with extensive practice on research grade equipment in parallel with the lecture topics. Though this new course was well received and met with success, the process of generating the course required development of a lot of the teaching resources myself, even as I grew in my own knowledge. Undergraduate crystallographic education is typically lacking in chemistry curricula,<sup>1</sup> and while there exist some online resources, I did not know where all of these were at the outset. As a result, some of the early iterations of my course had a number of errors stemming from my own lack of knowledge, and my own self-made, and occasionally flawed resources. It occurred to me early on that access to a database of teaching resources from existing experts would have eased my entry into crystallographic education, and made the first iterations of the course more successful. It has since been my interest to develop such a resource.

## A successful model: Inorganic VIPeR

A successful resource for inorganic chemical education, known as the Virtual Inorganic Pedagogical Electronic Resource (VIPeR),<sup>2</sup> is a collaborative educational effort from multiple institutions that provides free access to online teaching resources, online workshops, and forums. VIPeR has been funded by the National Science Foundation, and exists in partnership with the Division of Inorganic Chemistry of the American Chemical Society (ACS DIC). Perhaps most important is that users of VIPeR can download free teaching resources, and upload and share their own.



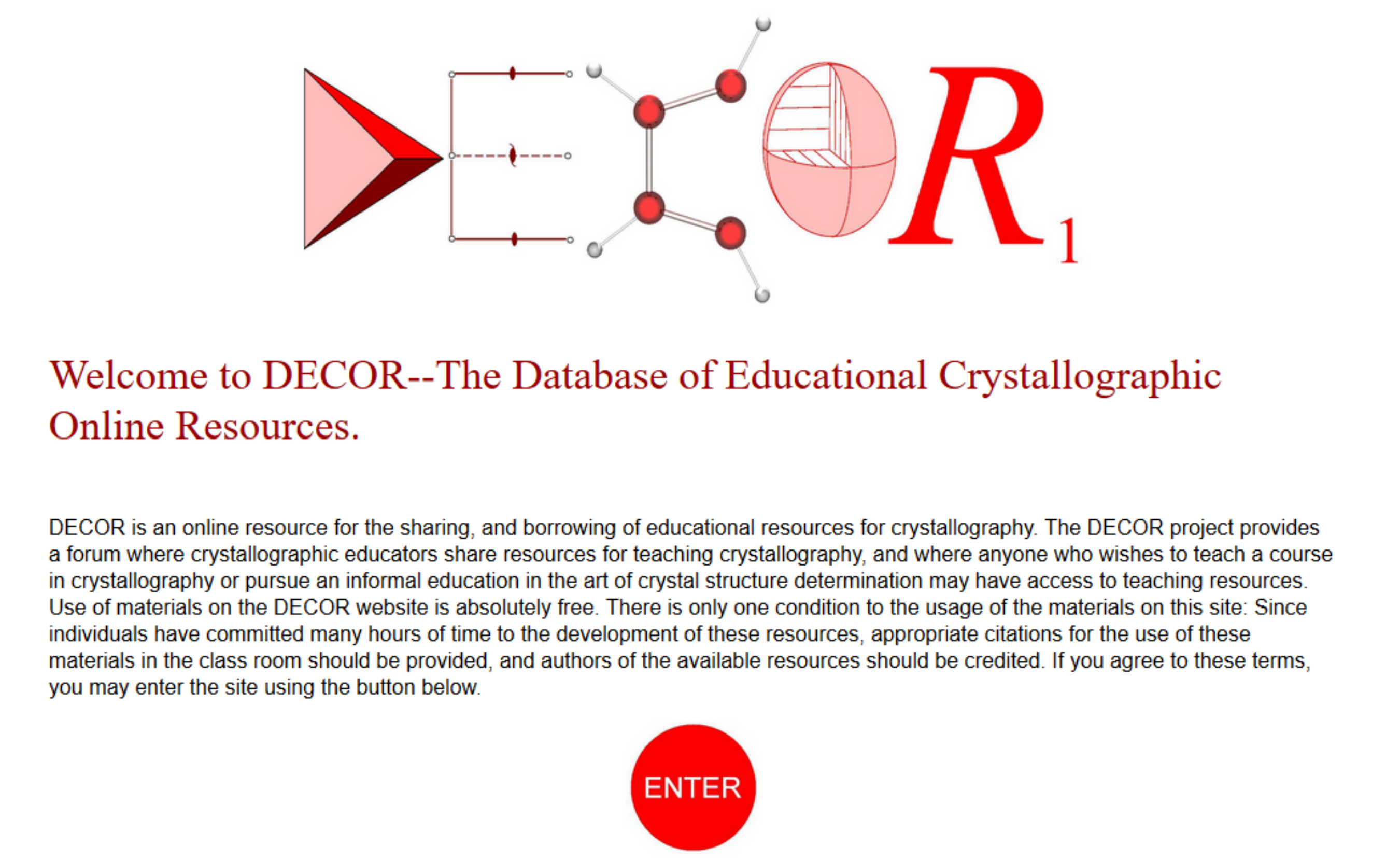
**Figure 1.** Screenshots from Inorganic VIPeR,<sup>2</sup> showing main page (left) and teaching resources (right).

## The Goal:

No analogous one-stop-shop for crystallographic teaching materials existed in 2009. A collection of websites hosted by various crystallographers were/are available, but word-of-mouth advice was needed to locate these resources. Obtaining examples of teaching materials from my crystallographic colleagues was also done in person on a one-on-one basis. The goal of DECOR<sup>3</sup> is the generation of just such a compendium of resources from the worldwide crystallographic community. The first version of DECOR is now available to the community, and was reviewed recently in *ACA Reflexions*.<sup>4</sup> The next steps are to expand participation from the worldwide community, and to develop a version of the site that is fully automated with respect to upload and organization of content.

## DECOR: Current release

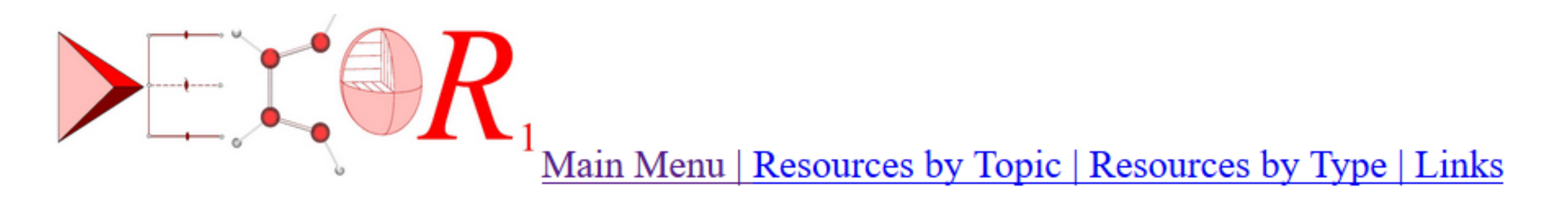
At present, DECOR features a respectable array of resources, which may be viewed by topic (e.g., “symmetry” or “reciprocal space”) or by type (e.g., homework problems, or animations). The greeting screen introduces the visitor to the site and its purpose:



**Figure 2.** Screenshot of the DECOR welcome page.

As the protection of intellectual property is of paramount importance, users of DECOR are required to agree (several times) to cite the creators of all work in any lecture notes or presentations that feature items from DECOR. At the outset, the user agrees to proper citation as a condition of entering.

Upon entering the site, the user is greeted by the main page, which offers a banner of options at the top, as well as a choice of several options for how to view DECOR's content:



## The Database of Educational Crystallographic Online Resources

### Resources by Topic

This menu organizes resources by lesson or topic. For example, you might surf to teaching aids on structure solution by Patterson methods, or anomalous scattering.

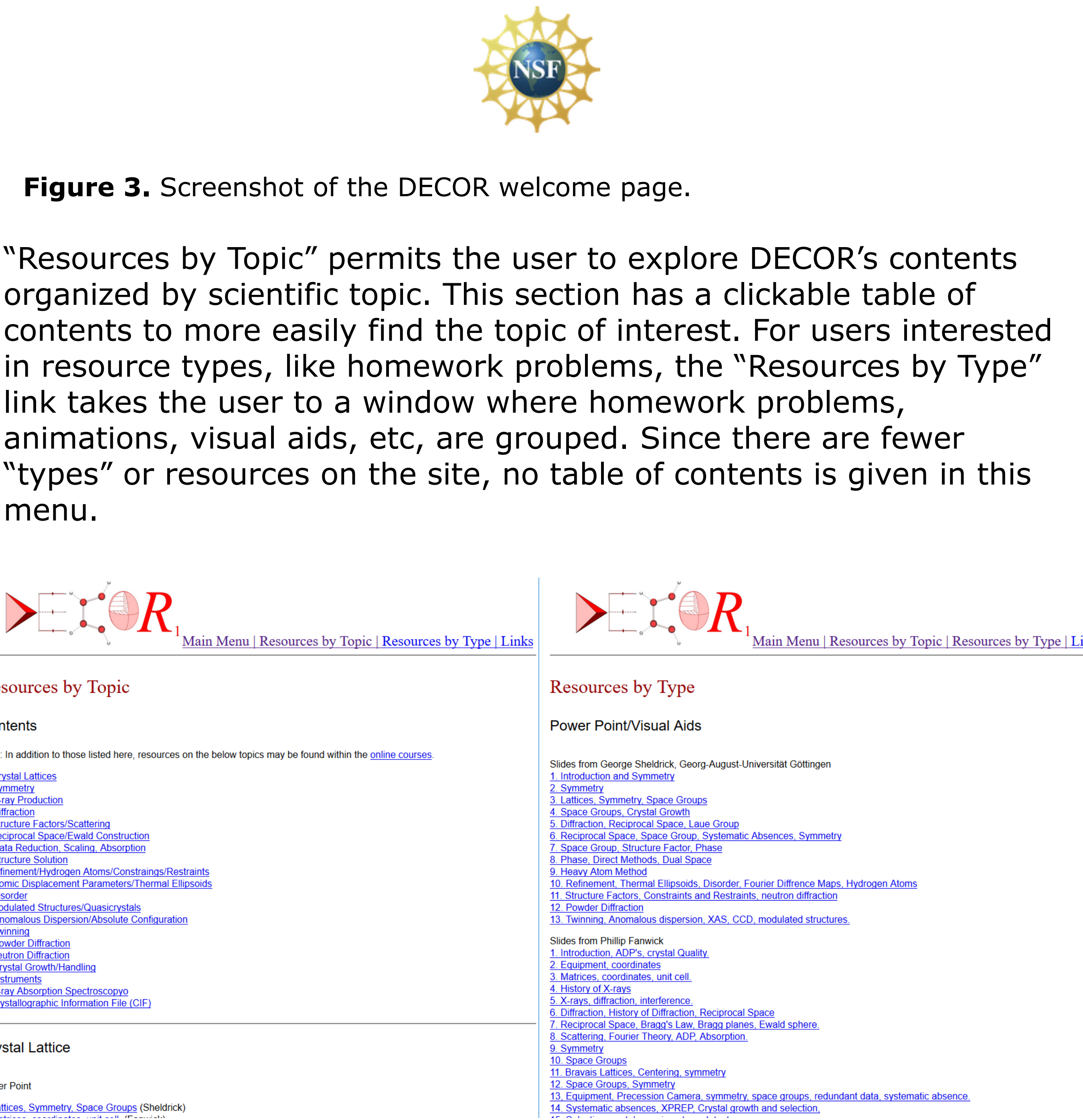
### Resources by Type

This menu displays teaching resources organized by type, in other words, you can surf to a menu of power point presentations, or homework problems.

The DECOR project is hosted by [Temple University, Department of Chemistry](#), 420 Beury Hall, 1901 N. 13th St. Philadelphia, PA 19122

To report problems, for more information, or to submit resources, please contact [Michael J. Zdilla](#)

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**Figure 4.** Screenshots of the DECOR resources organized by topic (left) and type (right).

Upon selecting a resource to download from the resource lists, the user is prompted once again to agree to cite the creator of that material. Upon clicking their agreement, the user's download begins.



**Figure 5.** Screenshot of the download confirmation page.

Finally, the links menu provides resources that are useful for the study of crystallography, but not necessarily focused on classroom education. Those websites that are educational in nature are also included in the lists of resources in the other menus to ensure users can locate them with ease.



## Links

Useful links for crystallography appear below.

1. International Union of Crystallography (IUCr)
2. IUCr CIF Checking Utility
3. Cambridge Crystallographic Data Centre (CCDC)
4. American Crystallographic Association (ACA)
5. SHELX (Crystallographic solution and refinement software)
6. PLATON - A multipurpose crystallographic tool
7. Mercury (Free Crystal Structure Viewer from CCDC)
8. Olex2 (Structure refinement and viewing software)
9. Ortep3 (Structure viewing and 3D rendering with POV-Ray)
10. JANA (Space group, structure solution and refinement for regular and modulated structures)
11. EnCIFer (CIF editing and checking software)
12. American Mineralogist Crystal Structure Database
13. Crystallography Open Database
14. Protein Data Bank (PDB)
15. Bilbao Crystallographic Server
16. Molecular Structure Laboratory Education Page, University of Wisconsin
17. Space group tables and diagrams from U. London
18. Crystal Growing Guides from Paul Boyle

**Figure 6.** Screenshot of the links page.

## DECOR: What's next?

- **Expanding the database: *Do you teach a crystallography course and have your own resources?*** I would love to add your materials to DECOR. I can be contacted at [mzdilla@temple.edu](mailto:mzdilla@temple.edu)
- **Automating the site:** At present, I manually code the site, and upload each resource, and generate a separate download page for each item. I also manually sort resources into categories. A component of a new NSF grant is to develop an automated “wiki-style” site, much like what Inorganic VIPeR<sup>2</sup> uses, so that users of DECOR directly upload and categorize their own content. They also can make changes to their own user profiles (e.g., institution) in case they have changes in status or address requiring changes in citation information. We are now partnering with the CCDC who have agreed to host the site. We are working with Yinka Olatunji-Ojo and Suzanna Ward to migrate the site to CCDC servers and then to begin development of an automated wiki-style database format that lets users and partners update and upload their own content.
- **Partnerships:** Inorganic VIPeR<sup>2</sup> is not a one-man effort, but rather an expansive project spanning multiple involved faculty and institutions. Further, the partnership with a professional society (ACS DIC) has been lucrative. I am interested in adopting this model by partnering with other individuals and organizations interested in helping to shape the future of the site.

## Acknowledgment of Funding

The current version of DECOR was funded in part by an NSF-CAREER award (CHE-1254545) that provided summer salary to work on the website and on the acquisition of material. A new award (CHE-1800105) will partially support efforts to generate an automated version of the site.

## References

<sup>1</sup>Fanwick, P.E. Observations on Crystallographic Education. *Annual Reports on Computational Chemistry*. **2007**, 3, 85-98.

<sup>2</sup>The Virtual Inorganic Pedagogical Electronic Resource: VIPeR: <https://www.ionicvipr.org/>

<sup>3</sup>The Database of Educational Crystallographic Online Resources: DECOR: <https://decor.cst.temple.edu>

<sup>4</sup>Vinokur, Anastasiya. Review: DECOR: The Database of Educational Crystallographic Online Resources. *ACA Reflexions*. **2016**, 3, 48.