

*Exploring the Ontology Landscape for Catalysis Research Data*

# **voc4cat\* - The NFDI4Cat service for collaborative management of terms in the field of catalysis**

Dr. David Linke

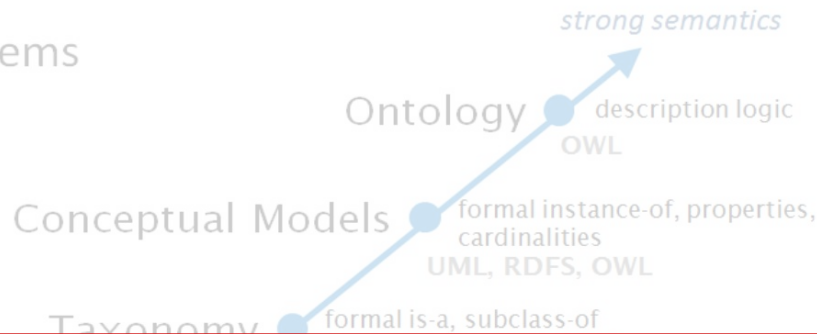
ADCR 2023, 2023-11-03



## Semantic Spectrum

of Knowledge Organization Systems

Intermediate deliverable  
**SKOS = Simple Knowledge Organization System**



- Task-force of domain experts collected ~2500 concepts related to homogeneous, heterogeneous catalysis, bio-catalysis and reaction engineering.
- **SKOS-related tools were found to be insufficient for collaborative development, especially if non-experts are involved.**



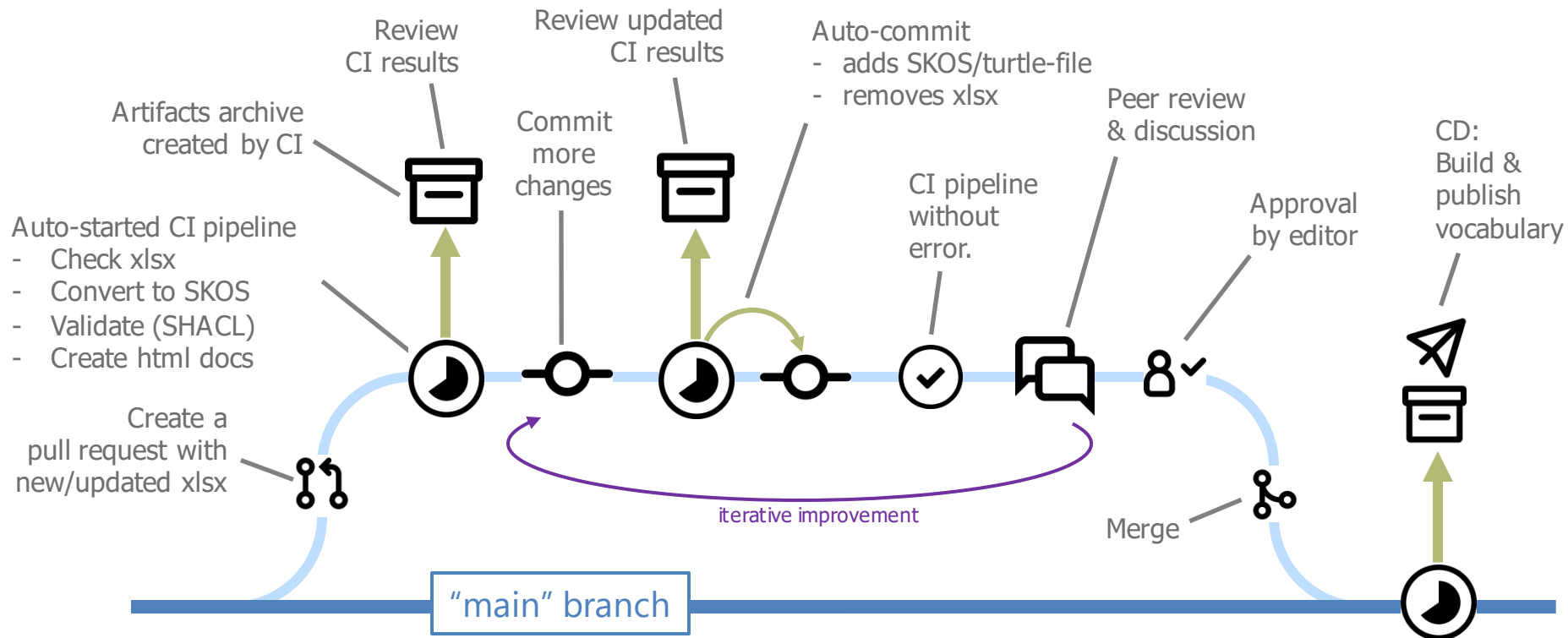
# Idea: Open-Source inspired Contribution Workflow

Libniz

...combined with Excel/xlsx as familiar user interface.

Concepts*								
Concept IRI*	Preferred Label*	Pref. Label Language Code	Definition*	Def. Language Code	Alternate Labels	Children IRIs	Provenance*	Source Vocab URI
https://w3id.org/nfdi4cat/voc4cat_0000001	photocatalysis	en	A process which catalyzes a chemical reaction through the absorption of sufficient light energy by a photocatalyst.	en	photocatalytic reaction	https://w3id.org/nfdi4cat/voc4cat_0000002, https://w3id.org/nfdi4cat/voc4cat_0000084, https://w3id.org/nfdi4cat/voc4cat_0000087, https://w3id.org/nfdi4cat/voc4cat_0000003, https://w3id.org/nfdi4cat/voc4cat_0000016, https://w3id.org/nfdi4cat/voc4cat_0000045, https://w3id.org/nfdi4cat/voc4cat_0000004, https://w3id.org/nfdi4cat/voc4cat_0000006, https://w3id.org/nfdi4cat/voc4cat_0000014	0000-0002-6242-2167 Nikolaos G. Moustakas created the resource	
https://w3id.org/nfdi4cat/voc4cat_0000002	photocatalyst	en	A material that absorbs photons (light) of appropriate energy and initiates or accelerates a photochemical reaction, while it regenerates itself after each reaction	en	photocatalytic material	https://w3id.org/nfdi4cat/voc4cat_0000016, https://w3id.org/nfdi4cat/voc4cat_0000045, https://w3id.org/nfdi4cat/voc4cat_0000004, https://w3id.org/nfdi4cat/voc4cat_0000006, https://w3id.org/nfdi4cat/voc4cat_0000014	0000-0002-6242-2167 Nikolaos G. Moustakas created the resource	
https://w3id.org/nfdi4cat/voc4cat_0000003	semiconductor	en	A material with electrical conductivity between that of a conductor and an insulator.	en		https://w3id.org/nfdi4cat/voc4cat_0000005	0000-0002-6242-2167 Nikolaos G. Moustakas created the resource	
https://w3id.org/nfdi4cat/voc4cat_0000004	categories of semiconductors	en	Broad families of semiconduction materials (e.g., metal oxides) that can be used as photocatalysts in various applications.	en		https://w3id.org/nfdi4cat/voc4cat_0000005	0000-0002-6242-2167 Nikolaos G. Moustakas created the resource	
https://w3id.org/nfdi4cat/voc4cat_0000005	metal oxide	en	A chemical compound formed by the reaction of a metal with oxygen.	en		https://w3id.org/nfdi4cat/voc4cat_0000007, https://w3id.org/nfdi4cat/voc4cat_0000008, https://w3id.org/nfdi4cat/voc4cat_0000009	0000-0002-6242-2167 Nikolaos G. Moustakas created the resource	
https://w3id.org/nfdi4cat/voc4cat_0000006		en	Characteristic properties of a semiconductor used in the	en		https://w3id.org/nfdi4cat/voc4cat_0000007, https://w3id.org/nfdi4cat/voc4cat_0000008, https://w3id.org/nfdi4cat/voc4cat_0000009	0000-0002-6242-2167 Nikolaos G. Moustakas created the resource	

Concepts*			
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https://w3id.org/nfdi4cat/voc4cat_0000001	photocatalysis	en	A process which catalyzes a chemical reaction through the absorption of sufficient light energy by a photocatalyst.
https://w3id.org/nfdi4cat/voc4cat_0000002	photocatalyst	en	A material that absorbs photons (light) of appropriate energy and initiates or accelerates a photochemical reaction, while it regenerates itself after each reaction
https://w3id.org/nfdi4cat/voc4cat_0000003		en	

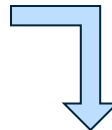


CI/CD = continuous integration/delivery realized with GitHub actions

- [voc4cat](#) is NFDI4Cat's vocabulary for catalysis-related disciplines
- Persistent identifiers managed via w3id.org
- Use of content negotiation to serve html for humans and turtle for machines



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- Documentation (html) hosted on gh-pages for all versions



The screenshot shows a web browser window with the URL <https://nfdi4cat.github.io/voc4cat/>. The page title is "Index of vocabulary versions". Below the title, it says "voc4cat CS". There is a vertical logo on the left that says "made by voc4cat 0.7.6". The main content area has a table with the following information:

Latest release	<a href="#">Documentation (HTML)</a>	<a href="https://w3id.org/nfdi4cat/voc4cat">https://w3id.org/nfdi4cat/voc4cat</a>
In development	<a href="#">Documentation (HTML)</a>	<a href="https://w3id.org/nfdi4cat/voc4cat/dev">https://w3id.org/nfdi4cat/voc4cat/dev</a>
	<a href="#">Spreadsheet file (xlsx)</a>	<a href="#">Documentation on GitHub (HTML)</a>

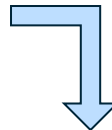
Below this table, there is a section titled "List of all releases" with the following information:

v2023-09-03	<a href="#">Documentation (HTML)</a>	<a href="https://w3id.org/nfdi4cat/voc4cat/v2023-09-03">https://w3id.org/nfdi4cat/voc4cat/v2023-09-03</a>
v2023-08-17	<a href="#">Documentation (HTML)</a>	<a href="https://w3id.org/nfdi4cat/voc4cat/v2023-08-17">https://w3id.org/nfdi4cat/voc4cat/v2023-08-17</a>

Link to most current xlsx file  
**Download and contribute!**



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- IDranges-config to reserve IDs by contributor (inspired by obofoundry)
- Repository configured to require approvals



Index of vocabulary versions

voc4cat <sup>CS</sup>

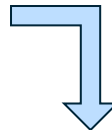
Latest release	<a href="#">Documentation (HTML)</a>	<a href="https://w3id.org/nfdi4cat/voc4cat">https://w3id.org/nfdi4cat/voc4cat</a>
In development	<a href="#">Documentation (HTML)</a>	<a href="https://w3id.org/nfdi4cat/voc4cat/dev">https://w3id.org/nfdi4cat/voc4cat/dev</a>
	<a href="#">Spreadsheet file (xlsx)</a>	<a href="#">Documentation on GitHub (HTML)</a>

List of all releases

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v2023-08-17	<a href="#">Documentation (HTML)</a>	<a href="https://w3id.org/nfdi4cat/voc4cat/v2023-08-17">https://w3id.org/nfdi4cat/voc4cat/v2023-08-17</a>



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- IDranges-config to reserve IDs by contributor (inspired by obofoundry)
- Repository configured to require approvals
- **zenodo** integration for new releases
- Listed in Bioregistry & **FAIRsharing.org** standards, databases, policies



Index of vocabulary versions

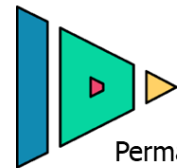
[voc4cat CS](#)

<b>Latest release</b>	<a href="#">Documentation (HTML)</a>	<a href="https://w3id.org/nfdi4cat/voc4cat">https://w3id.org/nfdi4cat/voc4cat</a>
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<b>v2023-08-17</b>	<a href="#">Documentation (HTML)</a>	<a href="https://w3id.org/nfdi4cat/voc4cat/v2023-08-17">https://w3id.org/nfdi4cat/voc4cat/v2023-08-17</a>





w3id.org

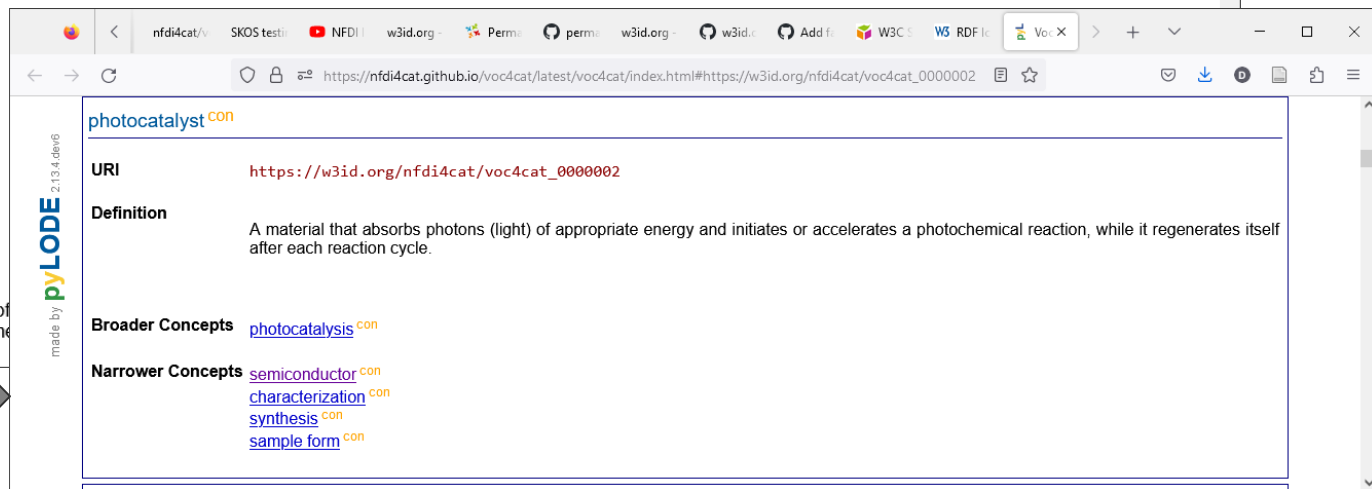
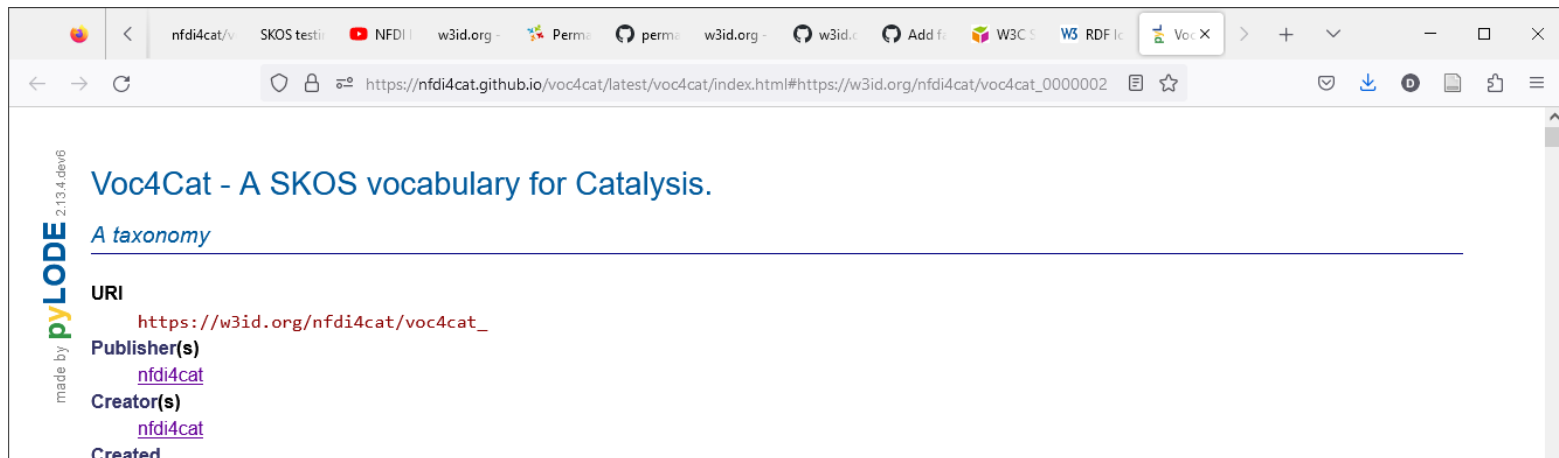
Permanent Identifiers for the Web

vocabularies > voc4cat > 0000002.ttl

```
1 PREFIX dcterms: <http://purl.org/dc/terms/>
2 PREFIX skos: <http://www.w3.org/2004/02/skos/core#>
3 PREFIX xsd: <http://www.w3.org/2001/XMLSchema#>
4
5 <https://w3id.org/nfdi4cat/voc4cat_0000002>
6   a skos:Concept ;
7   dcterms:identifier "voc4cat_0000002"^^xsd:token ;
8   dcterms:provenance "0000-0002-6242-2167 Nikolaos G. Moustakas created the resource"@en ;
9   skos:altLabel "photocatalytic material"@en ;
10  skos:broader <https://w3id.org/nfdi4cat/voc4cat_0000001> ;
11  skos:definition "A material that absorbs photons (light) of appropriate energy and
12  initiates or accelerates a photochemical reaction, while it regenerates itself after
13  each reaction cycle."@en ;
14  skos:inScheme <https://w3id.org/nfdi4cat/voc4cat_> ;
15  skos:narrower
16    <https://w3id.org/nfdi4cat/voc4cat_0000003> ,
17    <https://w3id.org/nfdi4cat/voc4cat_0000016> ,
18    <https://w3id.org/nfdi4cat/voc4cat_0000045> ,
19    <https://w3id.org/nfdi4cat/voc4cat_0000066> ;
20  skos:prefLabel "photocatalyst"@en ;
```

redirects to

In git we store one concept/collection per turtle file for better diffs.  
A file with all concepts in a single file is built as artifact in the merge pipeline.



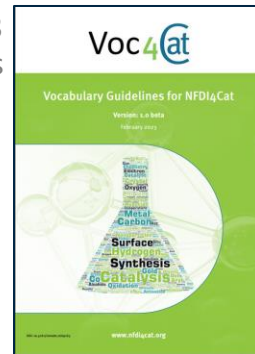
concept IRIs scroll to concept

DOI: 10.5281/zenodo.7669183  
Voc4cat Guidelines

All on GitHub organization  [nfdi4cat](https://github.com/nfdi4cat)

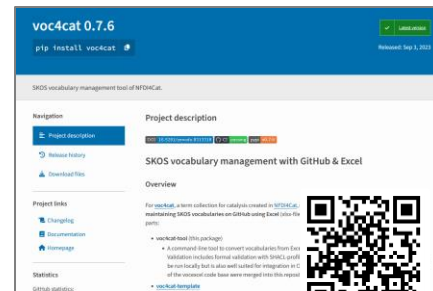
- NFDI4Cat's vocabulary for catalysis-related disciplines: [voc4cat](https://github.com/nfdi4cat/voc4cat)

- » Derived from and synced with voc4cat-template
- » Guidelines published



- Command line application: [voc4cat-tool](https://github.com/nfdi4cat/voc4cat-tool)

- » Convert between spreadsheet (xlsx) and SKOS/turtle
- » Validate spreadsheet (xlsx) or SKOS/turtle files



- Template for community-managed vocabularies: [voc4cat-template](https://github.com/nfdi4cat/voc4cat-template)

- » Reusable CI pipelines (GitHub action workflows) using voc4cat-tool



- Test-repository to play with: [voc4cat-playground](https://github.com/nfdi4cat/voc4cat-playground)