A Brief History of ChemistryFeaturization

(...and some lessons learned along the way)

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JuliaMolSim minisymposium

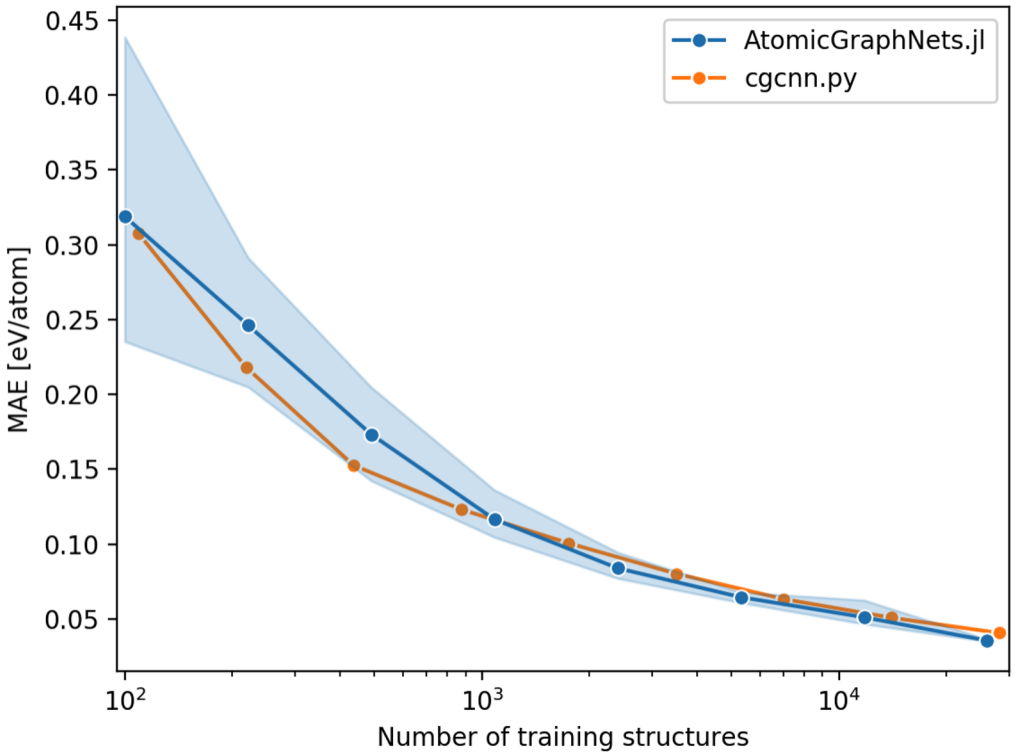
JuliaCon 2022

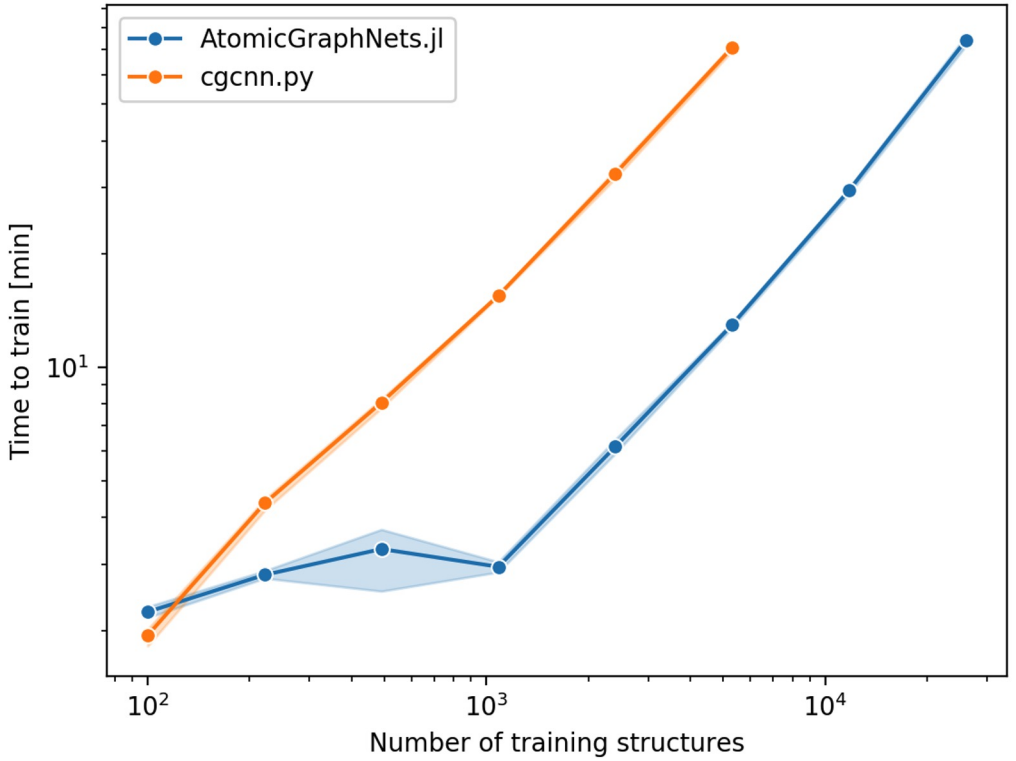

: rkurchin.github.io


: @rachel_kurchin

AtomicGraphNets.jl

- Built on Flux.jl, defines basic layers for convolution and pooling
- Competitive/superior performance relative to cgcnn.py:





Julia model = 21001 trainable params

Python model = 80833 trainable params

https://github.com/Chemellia/AtomicGraphNets.jl

today!

ChemistryFeaturization.jl is born

Jul ‘20

…out of frustration with standard approaches’ opacity and rigidity.

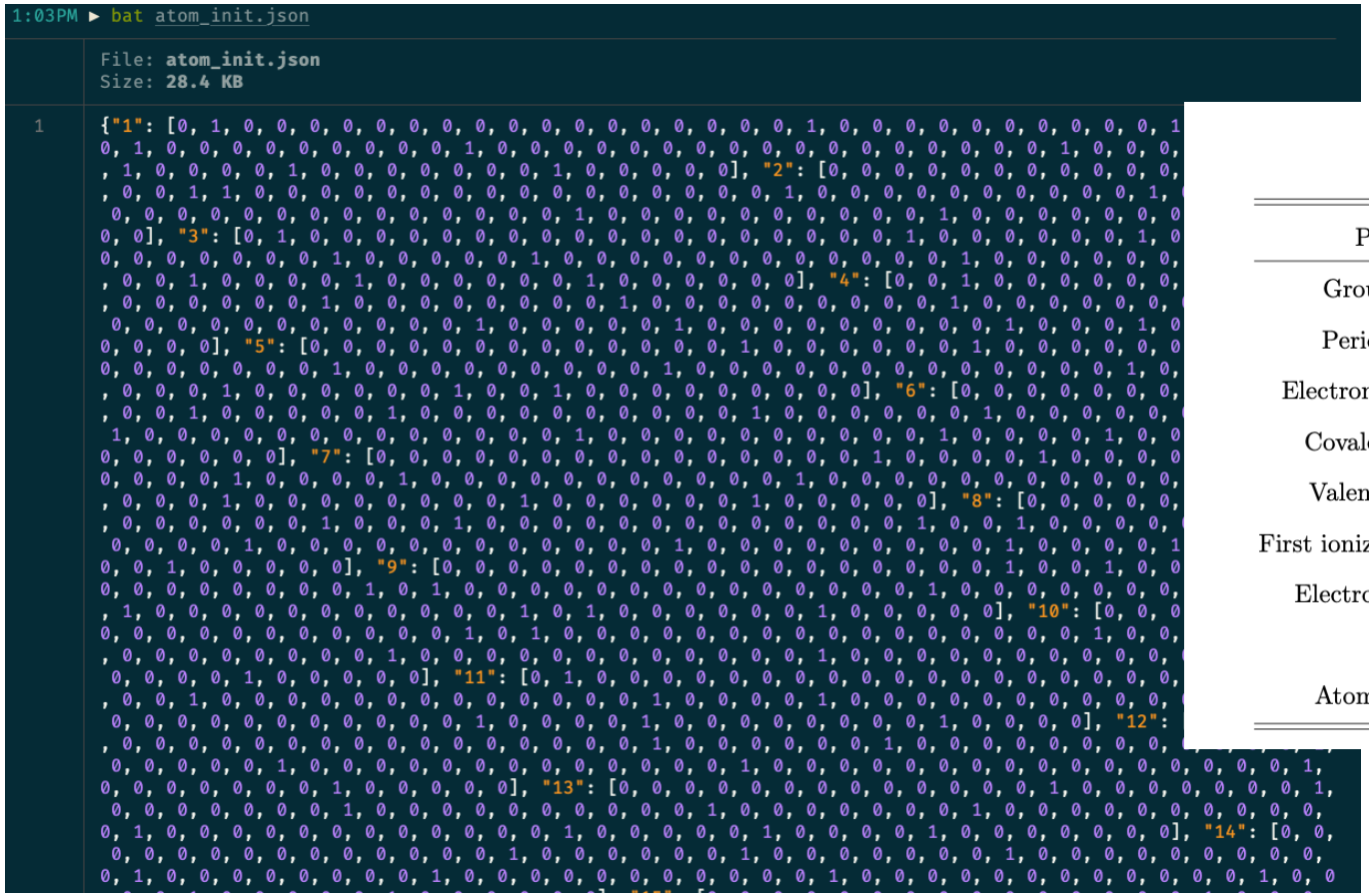


TABLE S2: Properties used in atom feature vector $\boldsymbol{v}_i$

Property	Unit	Range	# of categories
Group number	–	1,2, ..., 18	18
Period number	–	1,2, ..., 9[a]	9
Electronegativity[7, 8]	–	0.5–4.0	10
Covalent radius[3]	pm	25–250	10
Valence electrons	–	1, 2, ..., 12	12
First ionization energy[9][b]	eV	1.3–3.3	10
Electron affinity[10]	eV	-3–3.7	10
Block	–	s, p, d, f	4
Atomic volume[b]	cm^3/mol	1.5–4.3	10

today!

ChemistryFeaturization Design Principles

Jul '20

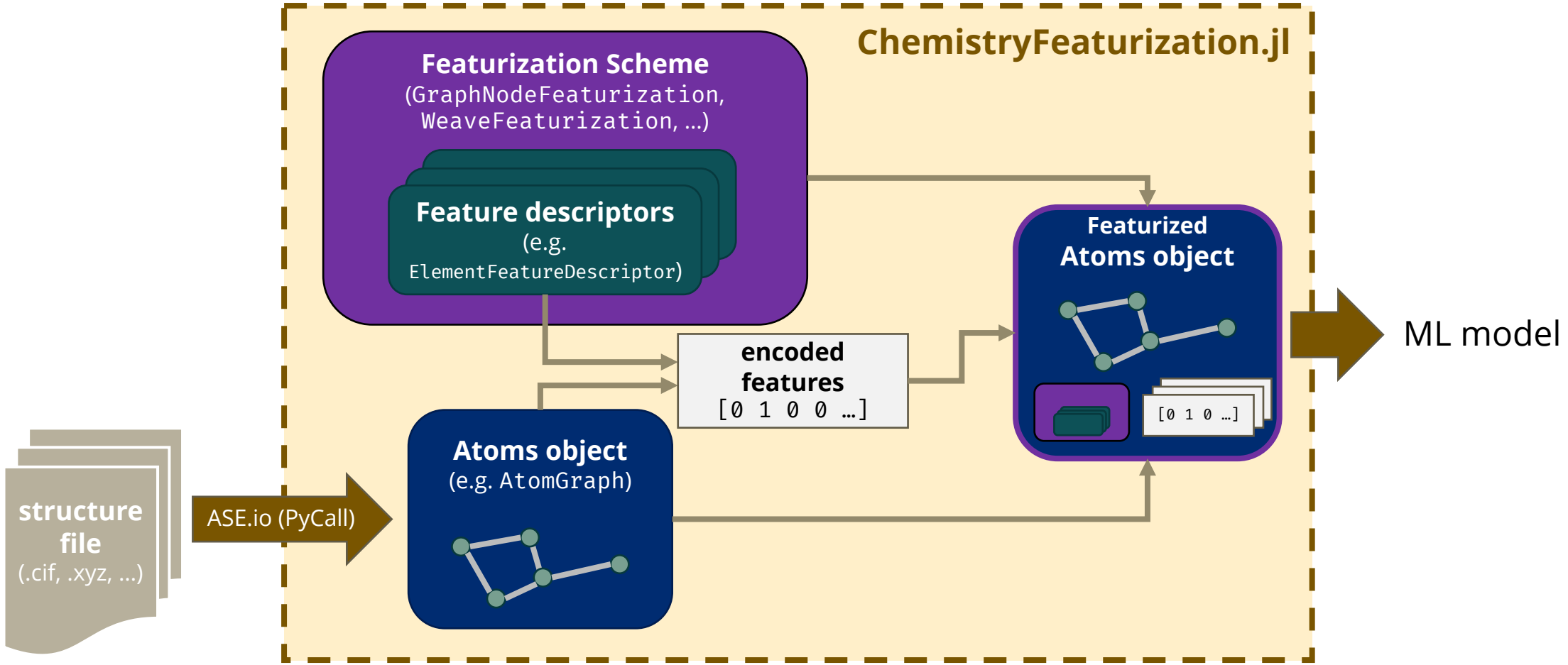
- Transparency: *what information am I encoding, and how?*
- Flexibility: *I want this feature (at this resolution) but not that one*
- Invertibility: *I want to be able to undo my feature encoding!*
- Versatility: *I'd like to use the same API for diverse atomic systems!*
- Extensibility: *…and it should be easy for me to make that happen!*

Concept: "one-stop-shop" for atomic representations, feature specification, encoding/decoding, providing standardized output types for ML models we build

today!

ChemistryFeaturization as of July 2020

Jul '20



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More support!

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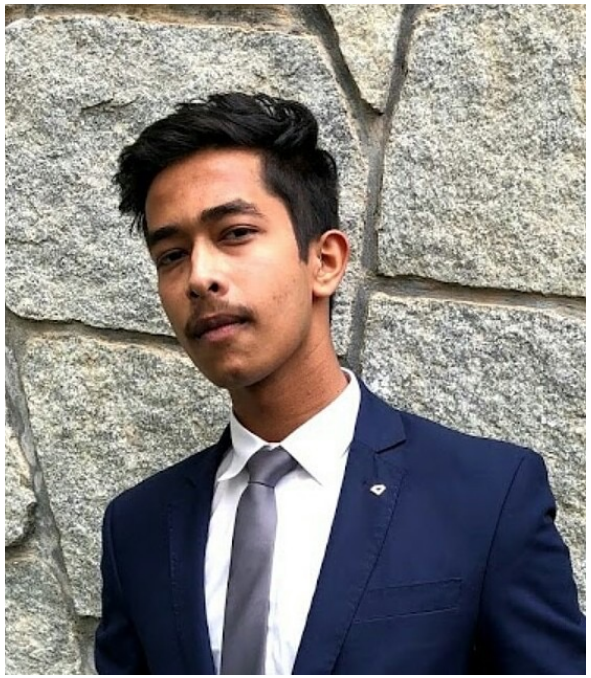
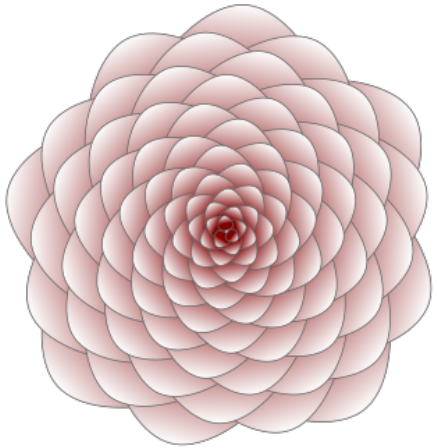
Nov ‘20

Jan ‘21



today!

Introducing…



Chemellia

May ‘21

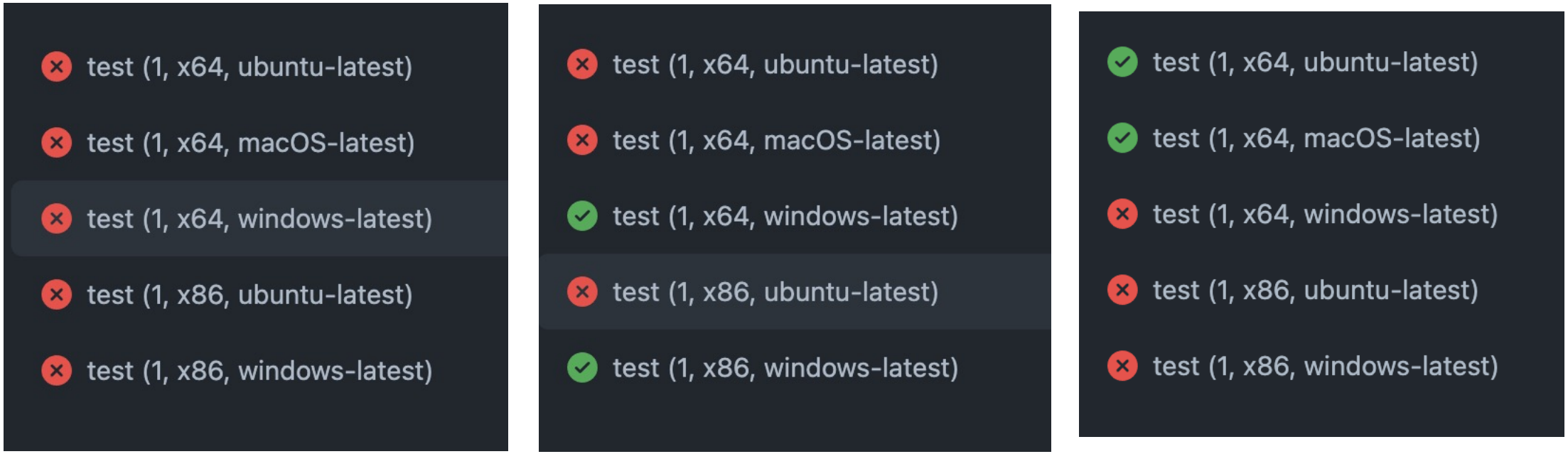
Ecosystem for machine learning with atoms encompassing ChemistryFeaturization, AtomicGraphNets, and more!

https://chemellia.org, https://github.com/Chemellia

today!

ChemistryFeaturization gets bloated...

A representative set of CI results as a PR progresses...



Nov '21

...mainly due to too many deps on other heavy/complicated packages like PyCall/Conda, etc.

today!

...and then slims down!

File: **Project.toml**

```
name = "ChemistryFeaturization"
uuid = "6c925690-434a-421d-aea7-51398c5b007a"
authors = ["Rachel Kurchin <rkurchin@cmu.edu>", "Anant Thazhema
version = "0.6.1"

[deps]
CSV = "336ed68f-0bac-5ca0-87d4-7b16caf5d00b"
Colors = "5ae59095-9a9b-59fe-a467-6f913c188581"
Compose = "a81c6b42-2e10-5240-aca2-a61377ecd94b
Conda = "8f4d0f93-b110-5947-807f-2305c1781a2d"
DataFrames = "a93c6f00-e57d-5684-b7b6-d8193f3e4
DataStructures = "864edb3b-99cc-5e75-8d2d-829cb
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GraphPlot = "a2cc645c-3eea-5389-862e-a155d00522
Graphs = "86223c79-3864-5bf0-83f7-82e725a168b6"
JSON3 = "0f8b85d8-7281-11e9-16c2-39a750bddbf1"
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MolecularGraph = "6c89ec66-9cd8-5372-9f91-fabc5
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```

✨ Interface-ify! ✨

File: **Project.toml**

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name = "ChemistryFeaturization"
uuid = "6c925690-434a-421d-aea7-51398c5
authors = ["Rachel Kurchin <rkurchin@cm
version = "0.7.0"

[deps]
AtomsBase = "a963bdd2-2df7-4f54-a1ee-49
CSV = "336ed68f-0bac-5ca0-87d4-7b16caf5
DataFrames = "a93c6f00-e57d-5684-b7b6-d
Flux = "587475ba-b771-5e3f-ad9e-33799f1
JSON3 = "0f8b85d8-7281-11e9-16c2-39a750
LinearAlgebra = "37e2e46d-f89d-539d-b4e
Serialization = "9e88b42a-f829-5b0c-bbe
SparseArrays = "2f01184e-e22b-5df5-ae63
```

Feb '22

today!

ChemistryFeaturization today!

- Mostly a lightweight interface with a few concrete functionalities exported
- Supports featurization of AtomsBase systems
- Separation of concerns between feature descriptors, codecs, featurization schemes, featurized structures

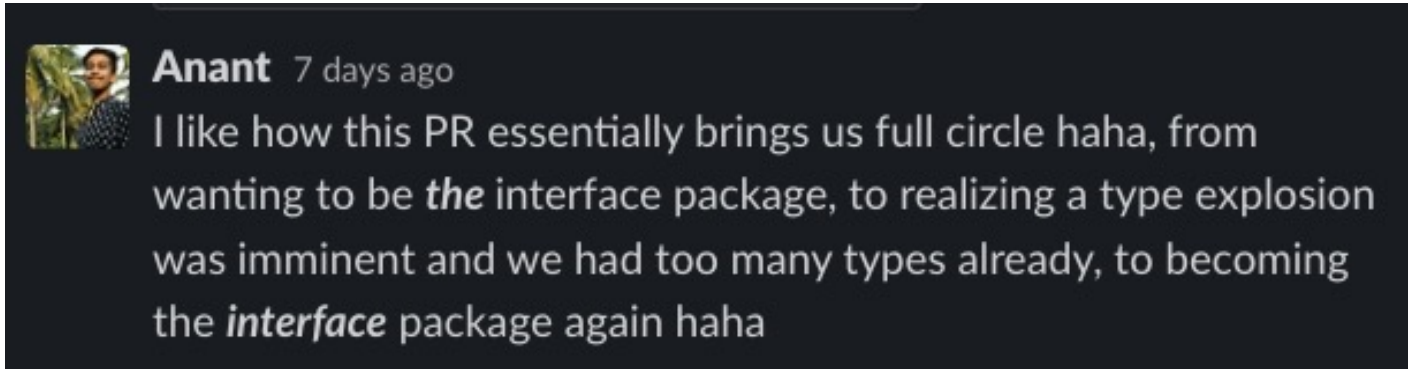
What's next?

Hopefully more active development again soon! 🤞
(We always welcome contributions!)

today!

Lessons Learned (and/or reinforced)!

- Julia interfaces are awesome



- Be willing to think big, but unashamed to start small
- Sometimes, writing up the description of your problem to send to the Julia Slack is enough for you to figure it out (#rubberduckcoding) but when it's not, they'll still answer your question within minutes

Acknowledgements!

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Google Summer of Code

@cormullion for the beautiful logo!