

# Lecture 03: Functions, interpolation, integration, differentiation

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# Reminder

- All homeworks, midterms, and finals will be Colabs
- You will have a week for each
- Late submissions are generally not a problem, but avoid accumulation
- Semester deadlines are final
- Don't hesitate to ask for help and additional explanations!

# This and that

- Any comments re first homework?
- Final project parameters:
  - Can be alternative to the final
  - Should meaningfully use optimization, Gaussian processes, or causal methods
  - Be connected to your own research
  - Ideally will become publication
- Some possibilities:
  - Explore molecular space towards candidates with specific functionality
  - Building workflow for materials optimization in automated synthesis
  - Causal analysis of the perovskite data base
  - ....

# Functions and spaces

- Our biggest strength – and weakness – is the intuition developed for the 3D Euclidean spaces
- Mathematicians has created large set of alternative spaces based on possible functional relationships and properties of objects
  - All real number
  - All integral numbers
  - All functions over unit interval
  - ... and many more
- In physical sciences, only a small subset of these is practically useful
- ... but these general principles are important to know!

# What is space?

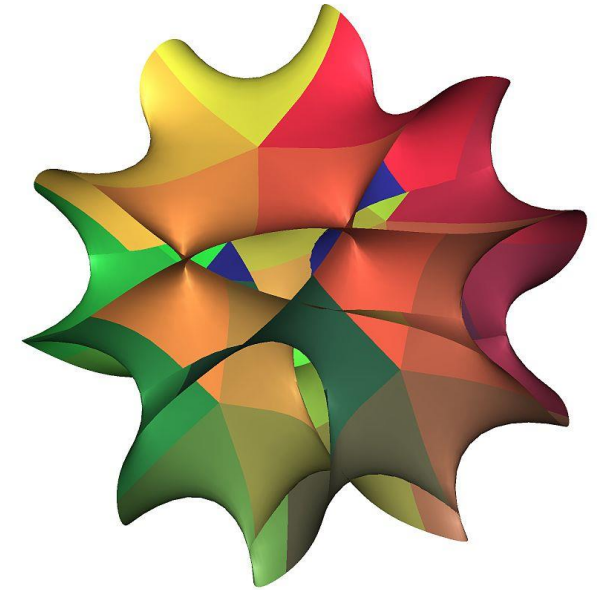
A space is a set with some added structure. It consists of selected mathematical objects that are treated as points, and selected relationships between these points.

The nature of the points can vary:

- elements of a set,
- functions on another space, or
- subspaces of another space.

The relationships between objects define the nature of the space.

Isomorphic spaces are considered identical, where an isomorphism between two spaces is a one-to-one correspondence between their points that preserves the relationships.



[https://en.wikipedia.org/wiki/Space\\_\(mathematics\)](https://en.wikipedia.org/wiki/Space_(mathematics))

[https://en.wikipedia.org/wiki/Calabi%E2%80%93Yau\\_manifold](https://en.wikipedia.org/wiki/Calabi%E2%80%93Yau_manifold)

# What is function?

In mathematics, a function from a set  $X$  to a set  $Y$  assigns to each element of  $X$  exactly one element of  $Y$ . The set  $X$  is called the domain of the function, and the set  $Y$  is called the codomain of the function.

We can define function by:

- Listing values
- Algebraic formulae
- Specified algorithm.
- ... and so on

## **Some function definitions:**

- $f$  is injective (or one-to-one) if  $f(a) \neq f(b)$  for any two different elements  $a$  and  $b$  of  $X$
- $f$  is surjective if its range  $X$  equals its codomain  $Y$ , i.e. for each element  $y$  of the codomain, there exists some element  $x$  of the domain such that  $f(x)=y$
- $f$  is bijective (or a one-to-one correspondence) if it is both injective and surjective. That is,  $f$  is bijective if, for any  $y \in Y$ , the preimage  $f^{-1}(y)$  contains exactly one element.

[https://en.wikipedia.org/wiki/Function\\_\(mathematics\)](https://en.wikipedia.org/wiki/Function_(mathematics))

# What should we look at practically?

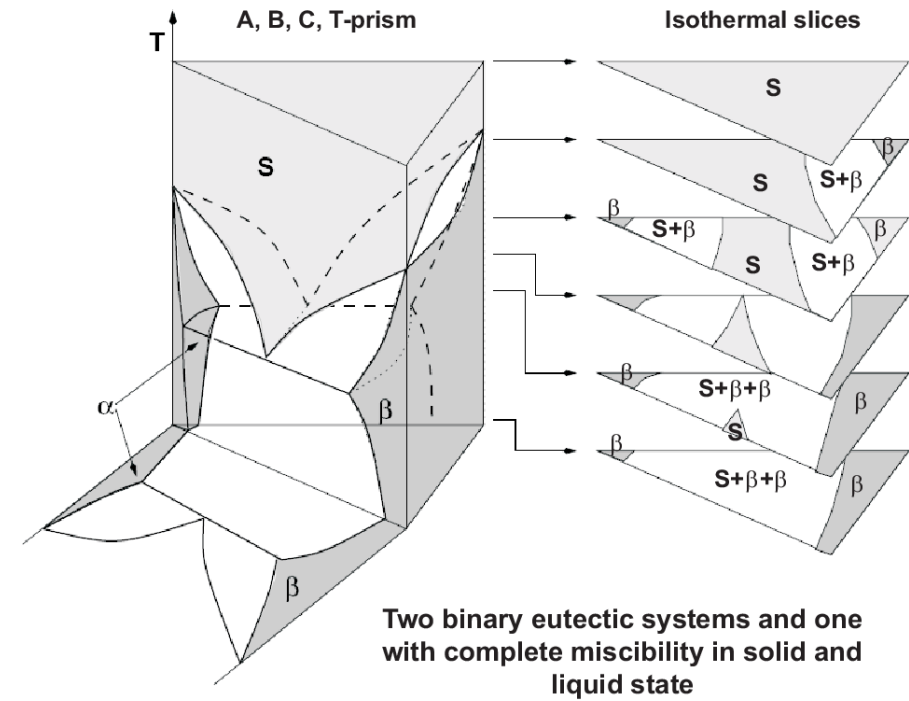
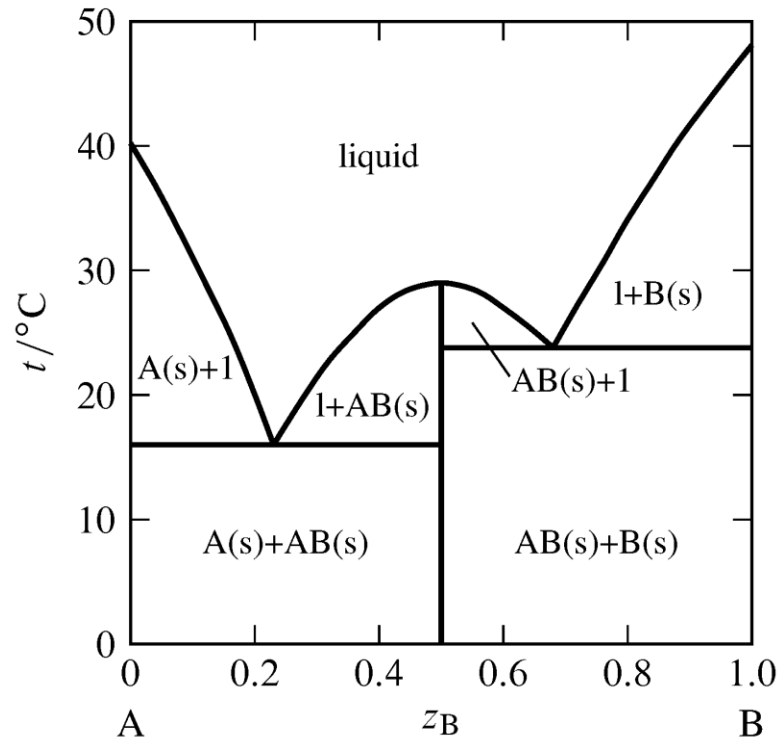
## **These are important:**

- Dimensionality
- Metrics (Distance Function)
- Continuity and Differentiability

## **These may be important:**

- Symmetry
- Topological Properties
- Inner Product (Hilbert Spaces)
- Manifold Structure

# Phase diagrams



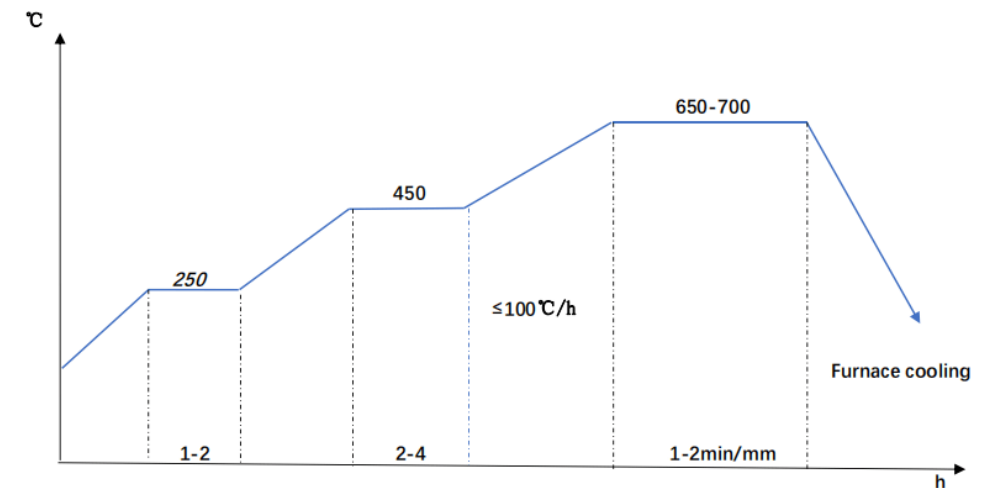
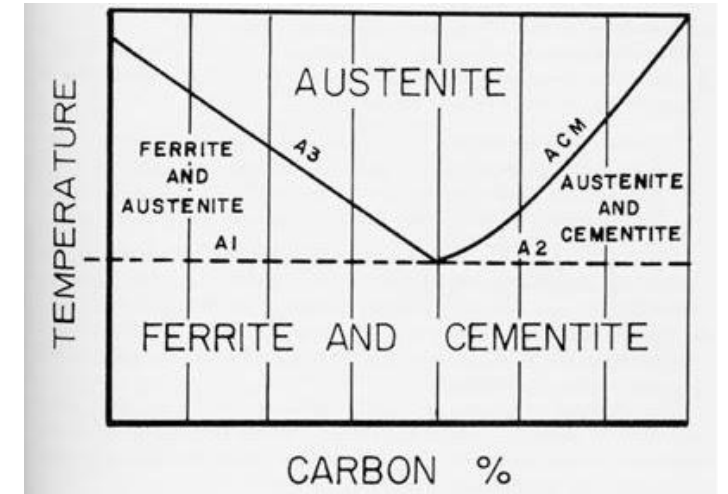
- What is the dimensionality of the parameter space?
- Is it differentiable?
- What is the function?
- Is it continuous?
- Is it differentiable

[13.2: Phase Diagrams- Binary Systems - Chemistry LibreTexts](https://www.tf.uni-kiel.de/matwis/amat/td_kin_ii/kap_1/backbone/r_se17.html)

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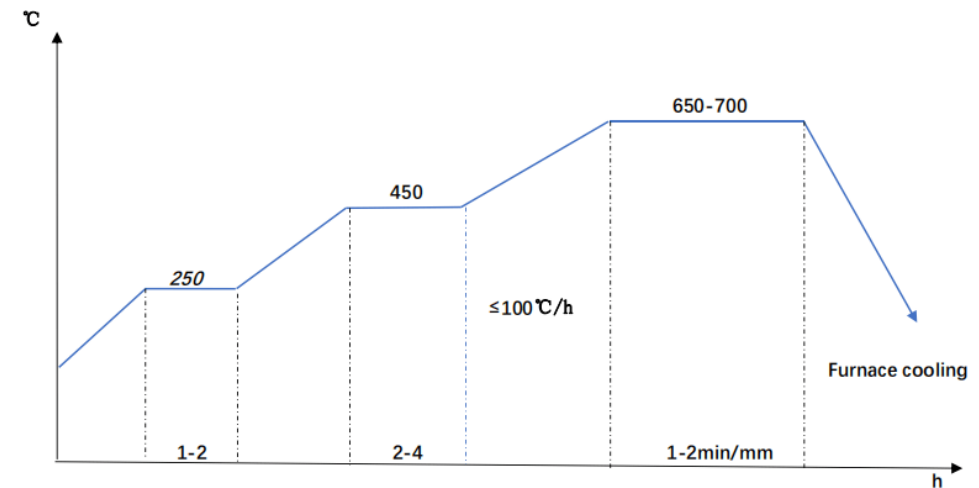
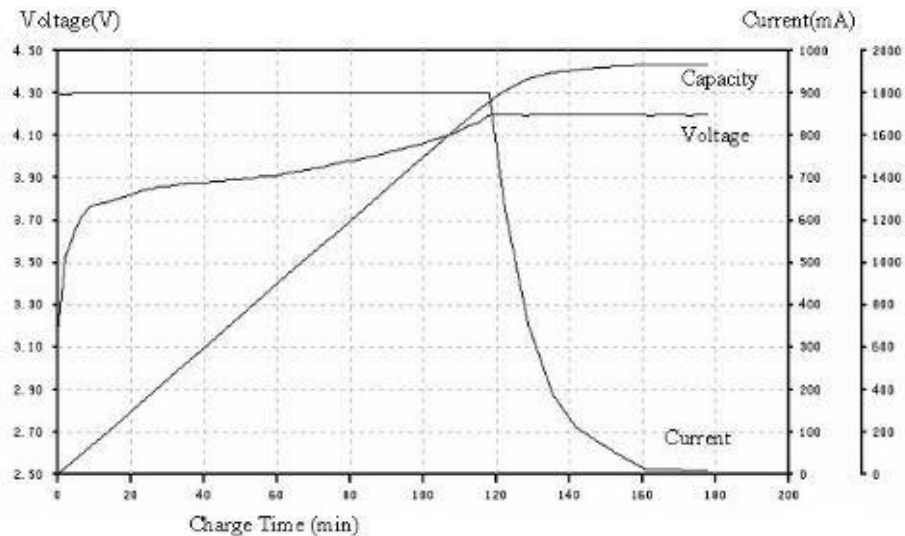


# Processing



# Processing

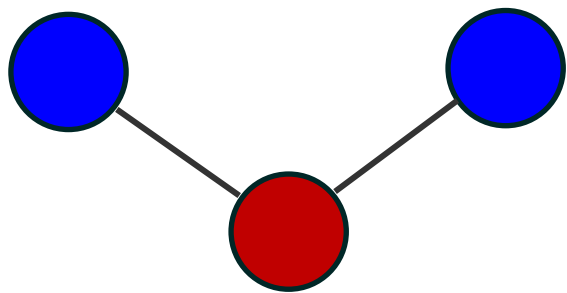
- Making steel – can be complicated and took a lot of time optimize
- Battery charging – fairly simple now, but obvious economic impact
- Annealing hybrid perovskite thin films
- Poling ferroelectric materials
- ... and so on



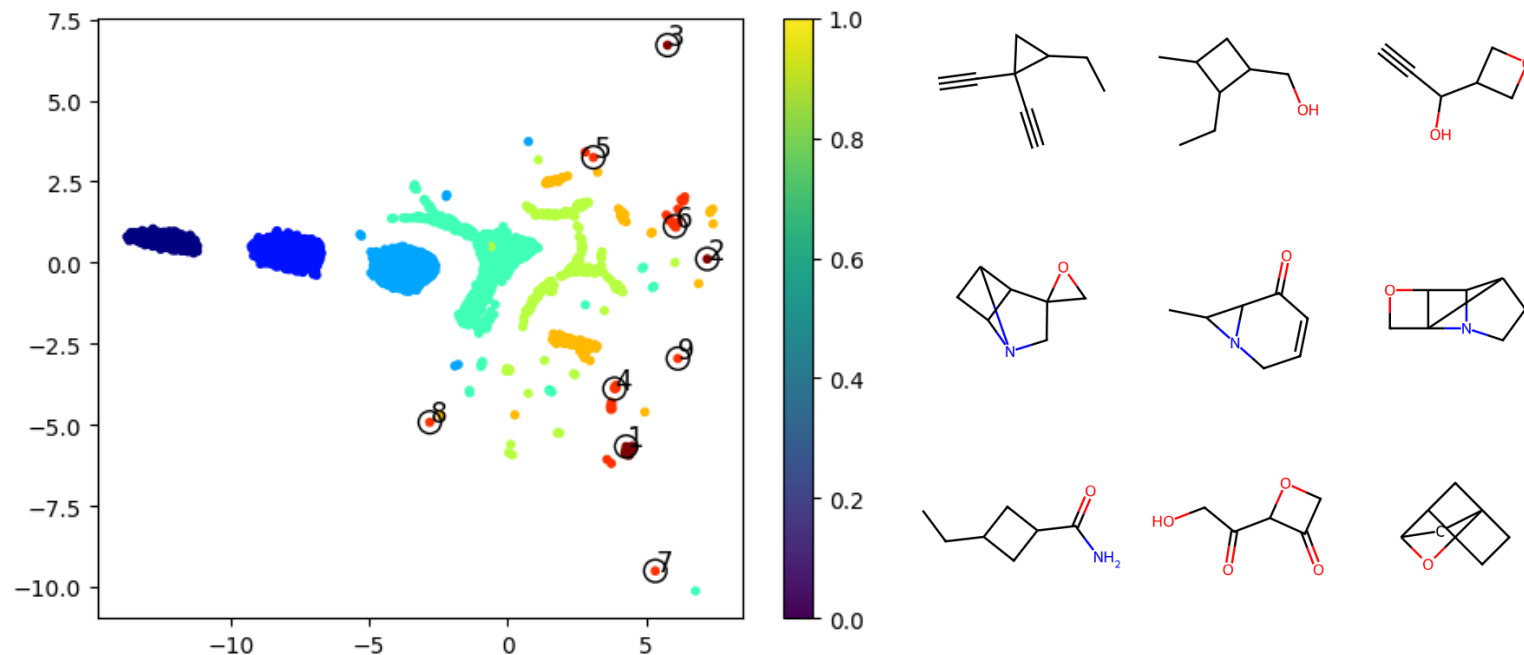
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# Molecular spaces

## Geometric space

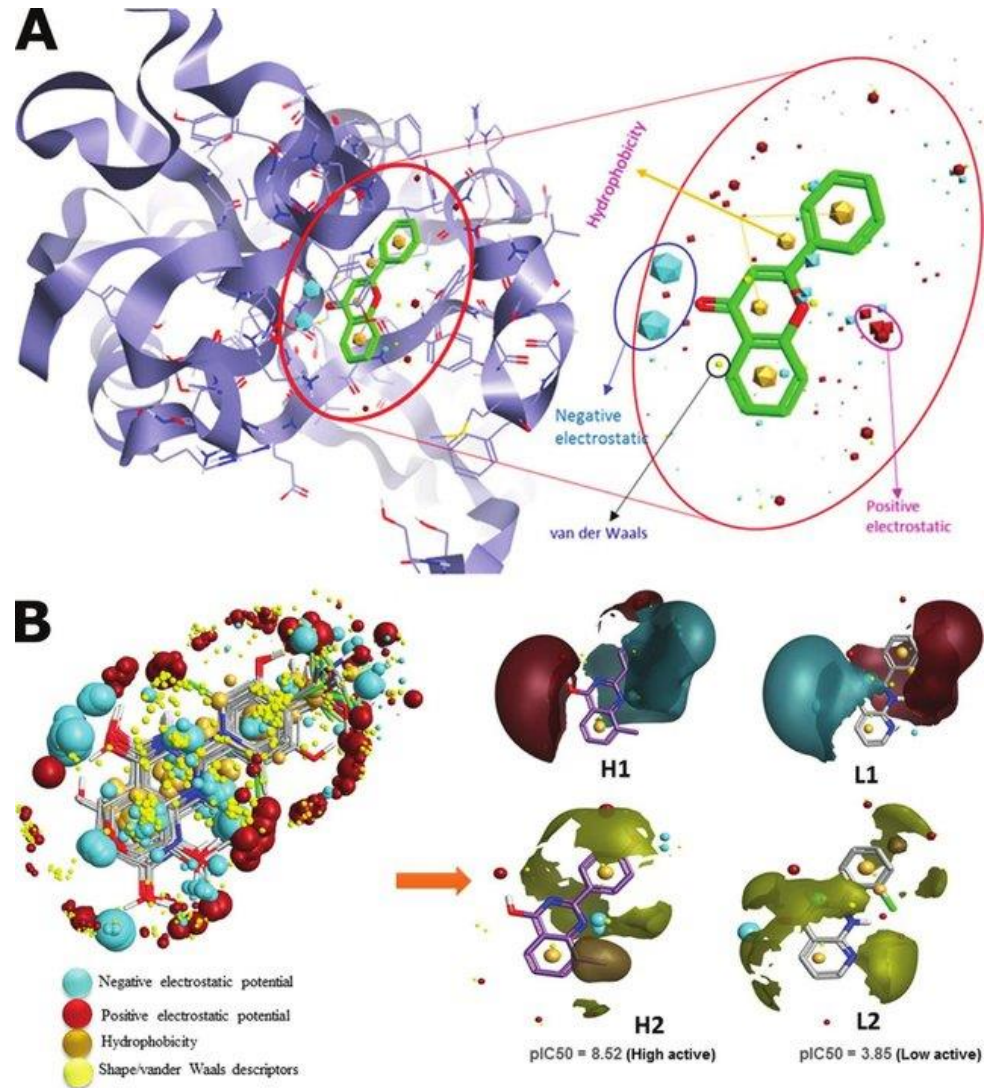


## Chemical space



- What is the dimensionality of the parameter space?
- Is it differentiable?
- What is the function?
- Is it continuous?
- Is it differentiable

# Structure–property relationships

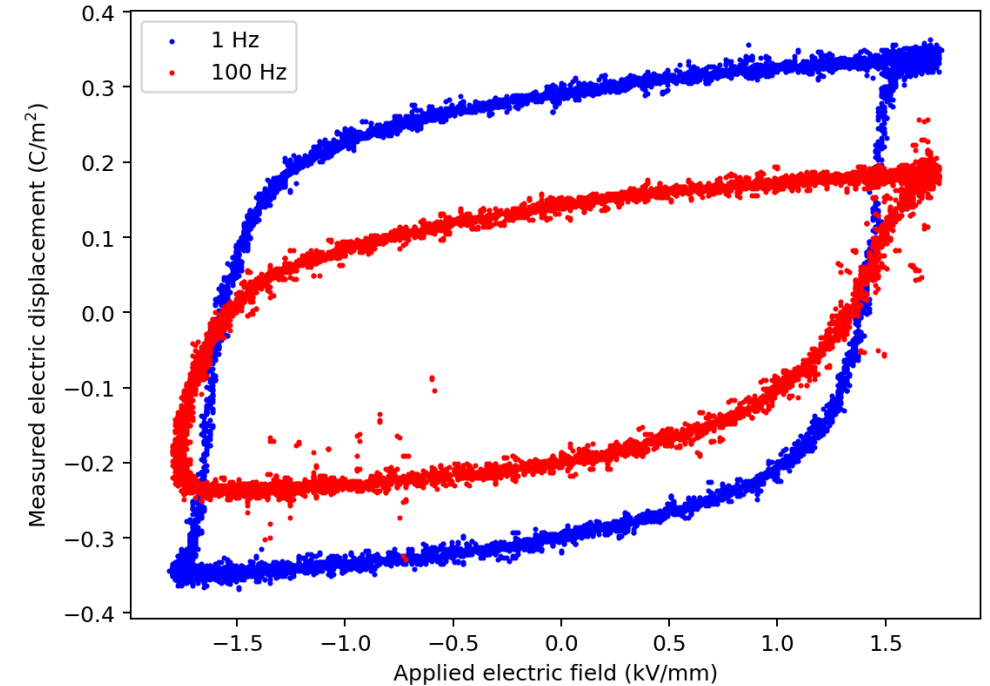
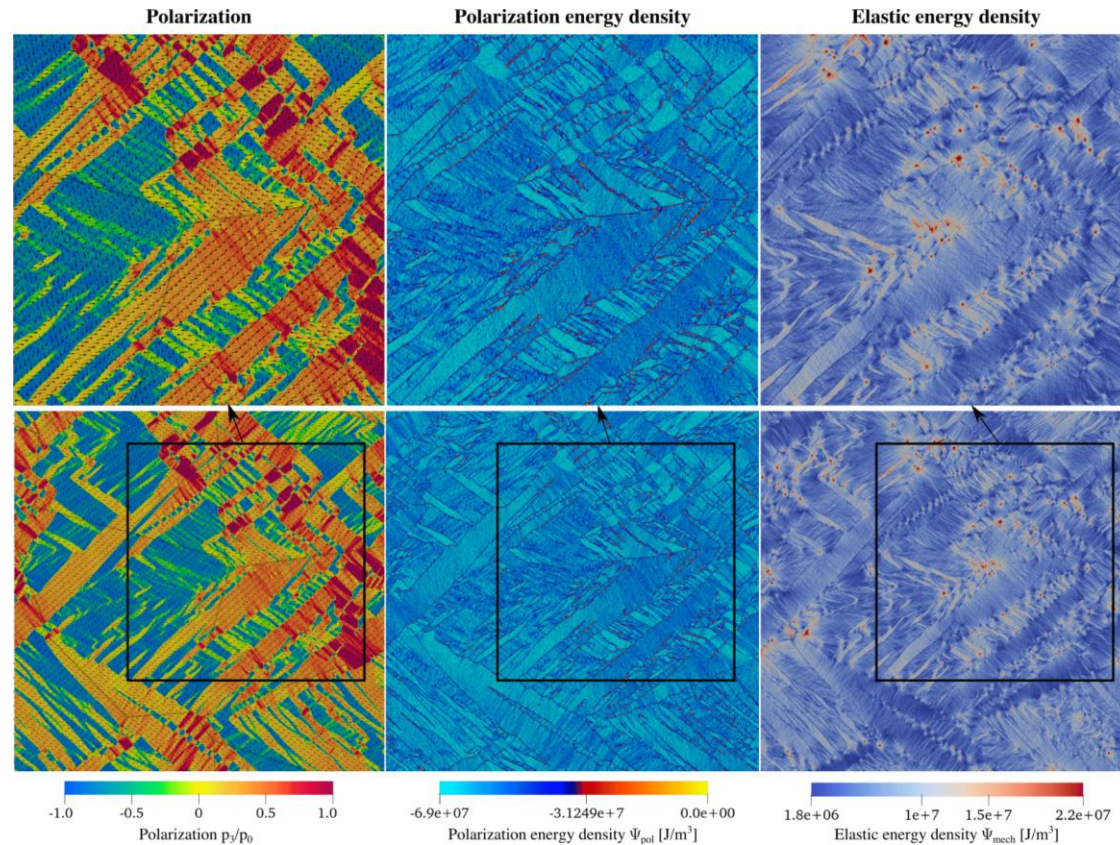


- What is the dimensionality of the parameter space?
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**Hint:** activity cliffs in quantitative structure-activity relations (QSAR)



# Structure–property relationships



- What is the dimensionality of the parameter space?
- Is it differentiable?
- What is the function?
- Is it continuous?
- Is it differentiable

# For each of these scenarios

- Can we interpolate?
- Can we differentiate?
- Can we integrate?
  - Phase diagram
  - Process trajectories
  - QASR
  - Hysteresis loops

# Off to Colab!