

# Descobrendo novos materiais usando Inteligência Artificial (e aprendendo algo novo no processo)

Daniel R. Cassar



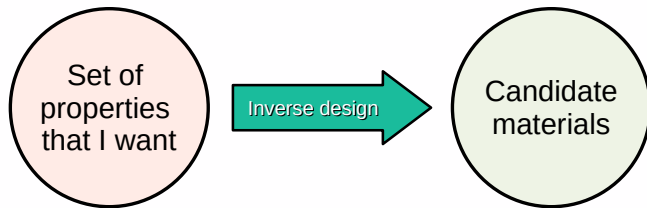
**CNPq**

MINISTÉRIO DA  
EDUCAÇÃO

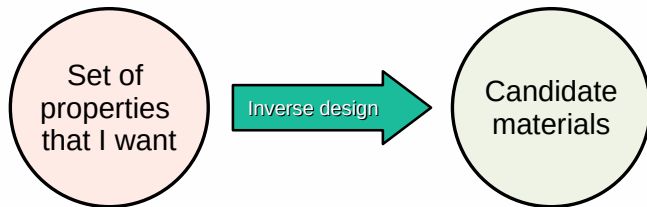
MINISTÉRIO DA  
CIÊNCIA, TECNOLOGIA  
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# Modelos preditivos e projeto inverso



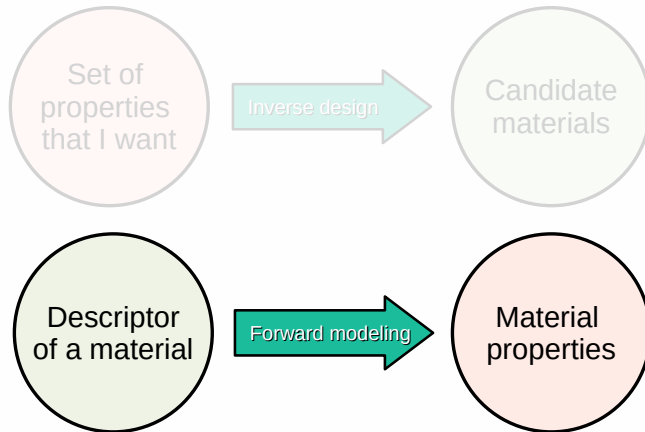
# Modelos preditivos e projeto inverso



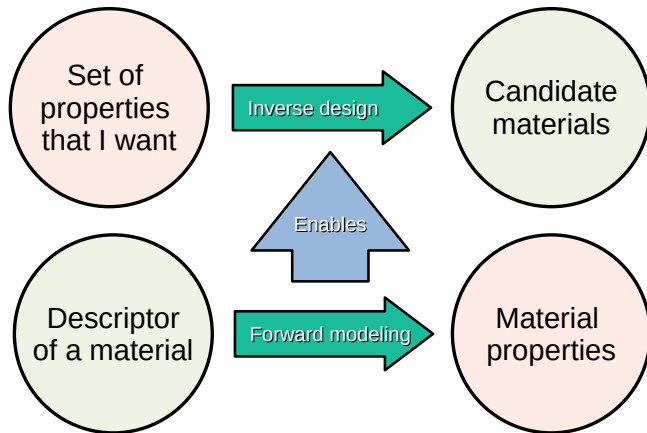
There are no physical models to solve the inverse design problem!

Solution: trial-and-error or optimization algorithms

# Modelos preditivos e projeto inverso



# Modelos preditivos e projeto inverso



# Modelos preditivos

## Descriptors

Chemical  
Composition

Processing  
Information

Microstructure

$f(x)$

## Target / Output

Property

Crystalline  
Structure

Microstructure

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# Modelos preditivos

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- Empirical Models
- Density Functional Theory
- Molecular Dynamics
- Kinetic Monte Carlo
- Reverse Monte Carlo
- Machine learning
- ...

$f(x)$

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Para ter o modelo preditivo por ML, precisamos de dados!



# Disponibilidade de dados — vidros inorgânicos

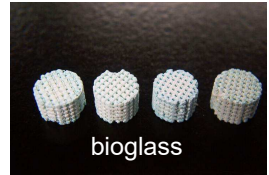
## SciGlass

The largest glass property database contains data for more than 420 thousand glass compositions including more than 18 thousand halide and about 38 thousand chalcogenide glasses. It provides also property predictions and calculations, help you solve R&D problems.

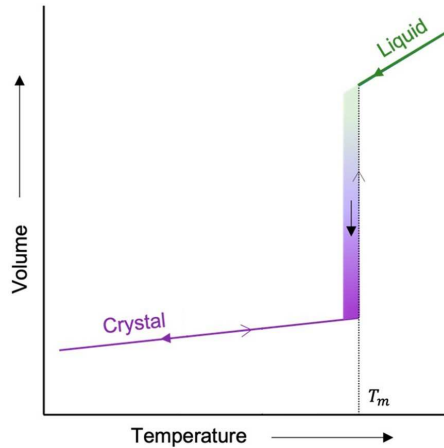
- Licença Open Database
- Mais de  $10^5$  entradas

<https://github.com/epam/SciGlass>

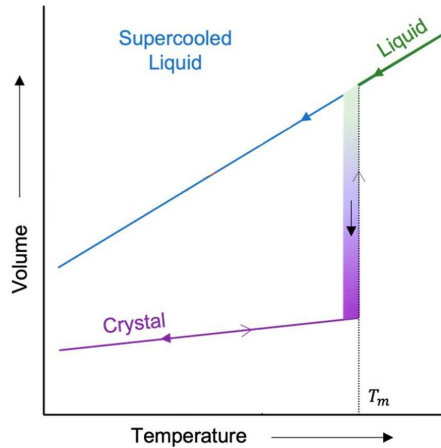
# A presença dos vidros na sociedade



# Formação de vidros

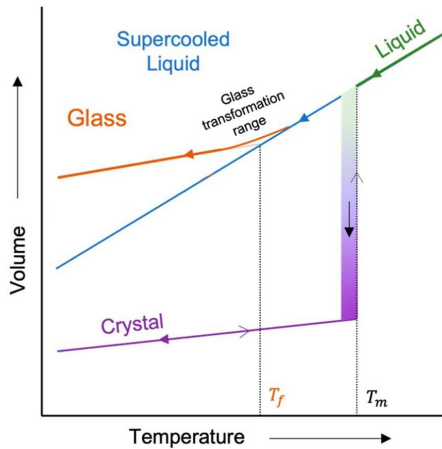


# Formação de vidros



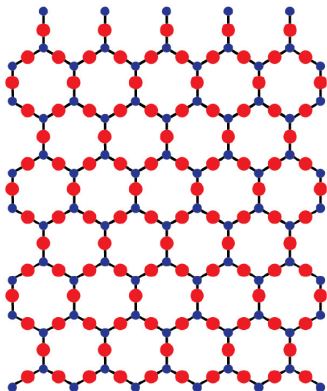


# Formação de vidros

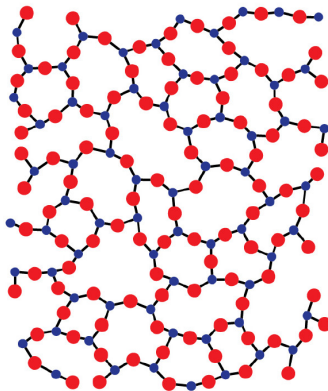


# Estrutura atômica

Cristal



Vidro ou líquido



# Da composição à aplicação — ciência dos materiais

- **Composition**



- **Processing**



- **Structure**



- **Properties**



- **Application**

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## How about Glasses?

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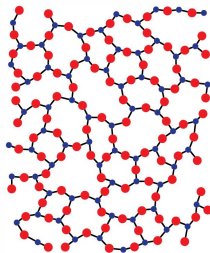


- **Properties**



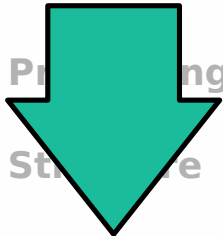
- **Application**

## How about Glasses?



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- **Application**

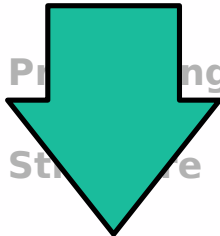
## How about Glasses?

(Cuidado! Isto é uma simplificação!!!)



# Da composição à aplicação — ciência dos vidros

- **Composition**



- Processing

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- **Properties**



- **Application**

**Opportunity!**

(Cuidado! Isto é uma simplificação!!!)

# Quer descobrir seu próprio vidro?

<https://github.com/drcassar/mlschool23>

<https://colab.research.google.com>