

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

Daniel R. Cassar



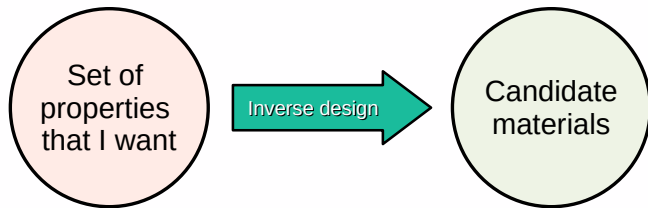
CNPq

MINISTÉRIO DA
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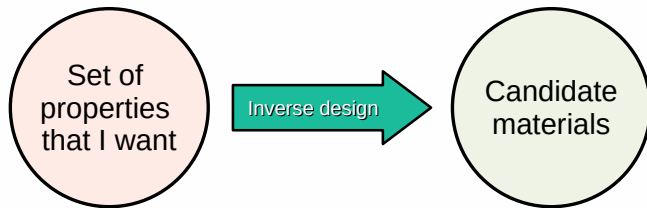
MINISTÉRIO DA
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Modelos preditivos e projeto inverso



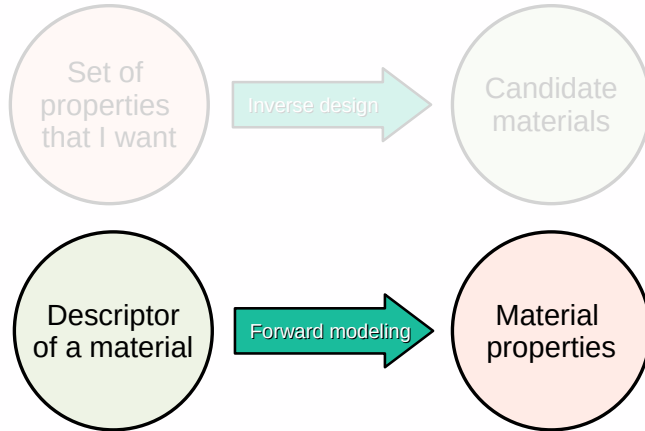
Modelos preditivos e projeto inverso



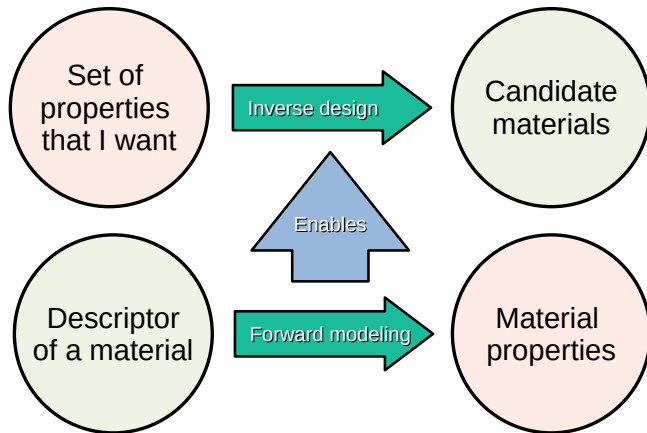
There are no physical models to solve the inverse design problem!

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

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Microstructure

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

$f(x)$

Target / Output

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Crystalline
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Microstructure

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



Disponibilidade de dados — vidros inorgânicos

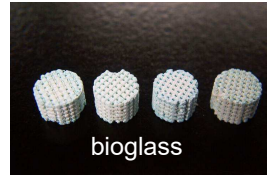
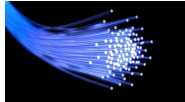
SciGlass

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

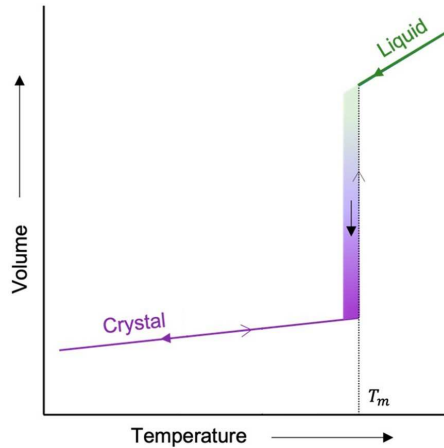
<https://github.com/epam/SciGlass>

A presença dos vidros na sociedade

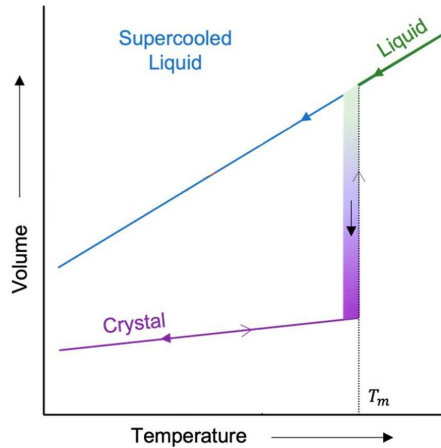


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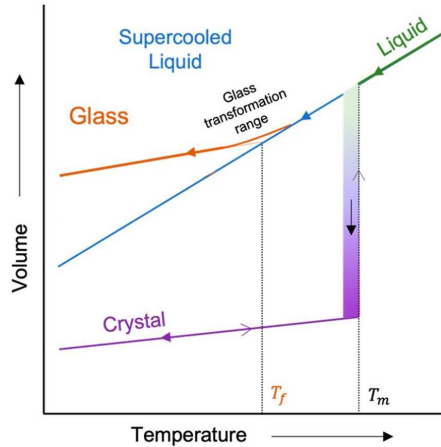
Formação de vidros



Formação de vidros

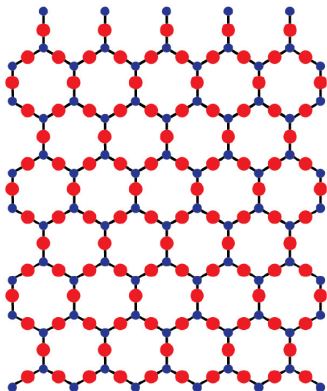


Formação de vidros

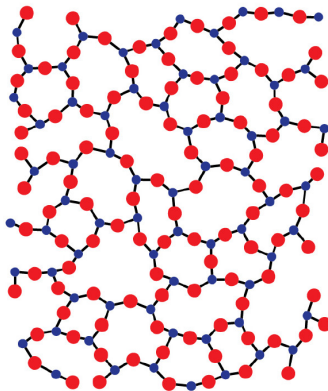


Estrutura atômica

Cristal



Vidro ou líquido



Da composição à aplicação — ciência dos materiais

- **Composition**



- **Processing**



- **Structure**



- **Properties**



- **Application**

Da composição à aplicação — ciência dos materiais

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How about Glasses?

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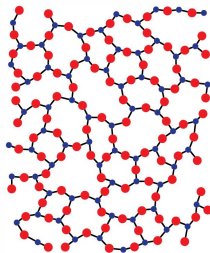


- **Properties**



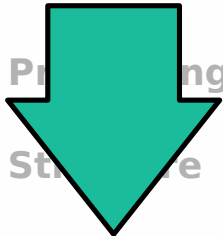
- **Application**

How about Glasses?



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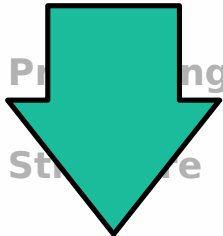
- **Application**

How about Glasses?

(Cuidado! Isto é uma simplificação!!!)

Da composição à aplicação — ciência dos vidros

- **Composition**



- Processing

- Structure

- **Properties**



- **Application**

Opportunity!

(Cuidado! Isto é uma simplificação!!!)

Quer descobrir seu próprio vidro?

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