Pesquisa e Desenvolvimento de Materiais Biocompatíveis para Eletrodos.

Atividade Contextualizada 10

INSTITUTO SANTOS DUMONT
ENSINO E PESQUISA

Discente: Gilberto Martins
Orientador: Edgard Morya

Sumário

Artigo Base

Machine Learning the Voltage of Electrode Materials in Metal-ion Batteries

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Link para o artigo: https://arxiv.org/pdf/1903.06813.pdf

Artigo Base

A Machine Learning Tool to Predict the Voltage of Cathode Materials in Batteries

Please enter the electrode specification below:

High ion concentration
Low ion concentration
Fraction of metal-ion
In high ion concentration, e.g. x/(x+3) for Li_xTiO_2
Type of metal-ion: Li
Crystal lattice type: cubic
Space group: 1
Submit Job

An example input:

For an intercalation reaction: $0.5Mg + Mg_{0.5}VO_3 = MgVO_3$
High ion concentration: MgVO3
Low ion concentration: Mg0.5VO3
Fraction of metal-ion: 0.20
Type of metal-ion: Mg
Crystal lattice type: orthorhombic
Space group: 63

Useful links:
1. Space group numbers and symbols
2. Crystal lattice type and space group

Authors: R. P. Joshi, J. Eickholt, L. Li, M. Fornari, V. Barone, J. E. Peralta

Please cite: Joshi *et al.*, ACS Appl. Mater. Interfaces 2019, 11, 20, 18494-18503, https://doi.org/10.1021/acsami.9b04933 [pdf]

Help: Don't know how to use the tool? Please read the Tutorial.

Contact: Veronica Barone at v.barone@cmich.edu, Rajendra Joshi at joshi1rp@cmich.edu

Caution: Model not trained with anode materials. Use tool with care for anodes.

Acknowledgements: Material Project Database

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Voltage Predictor

Job Details:

Predicted Voltage: 0.59 V
High ion concentration: MgCaNi4
Low ion concentration: Mg0.5CaNi4
Fraction of metal-ion: 0.2
Type of metal-ion: Mg
Crystal lattice type: hexagonal
Space group: 194

Submit another job.

Link: https://machine.lea.rning.dev/battery/voltage_predictor/index.php

Introdução

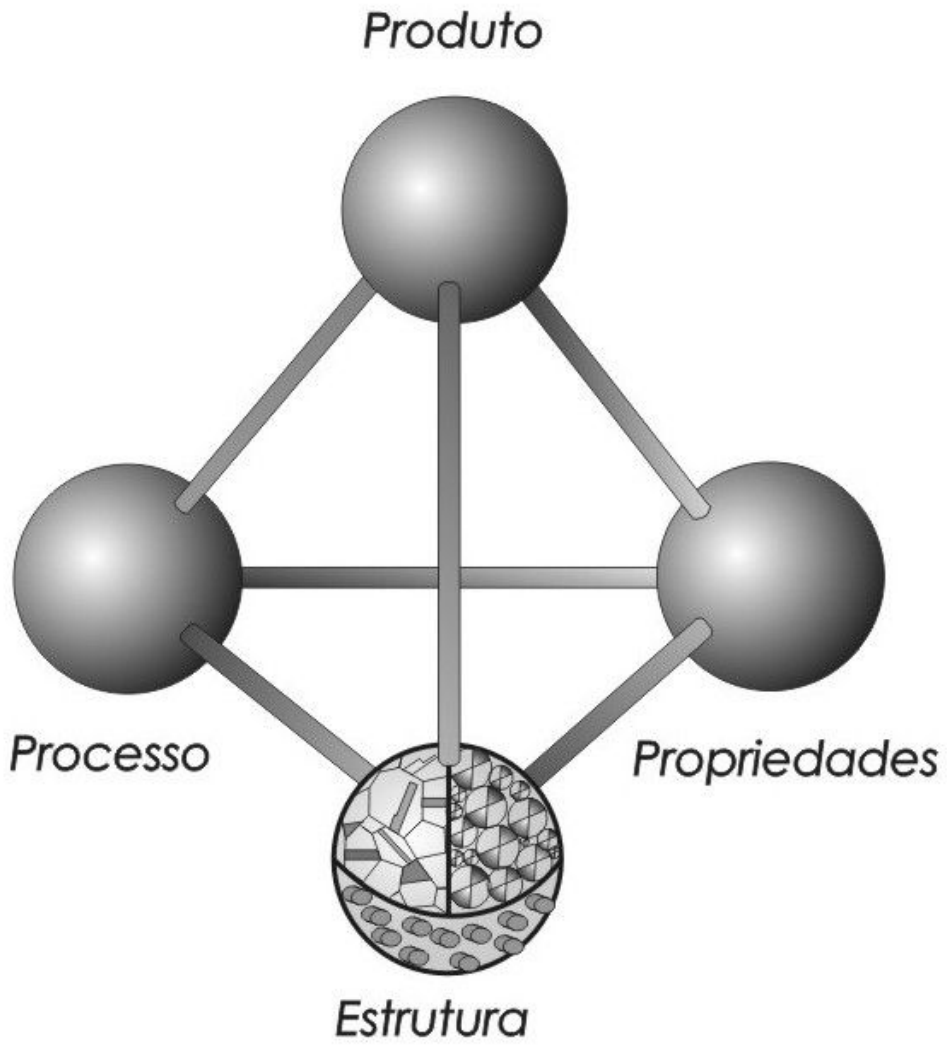


Figura 1 - Tetraedro de Ciência dos Materiais.
Fonte: Callister 8ªed.

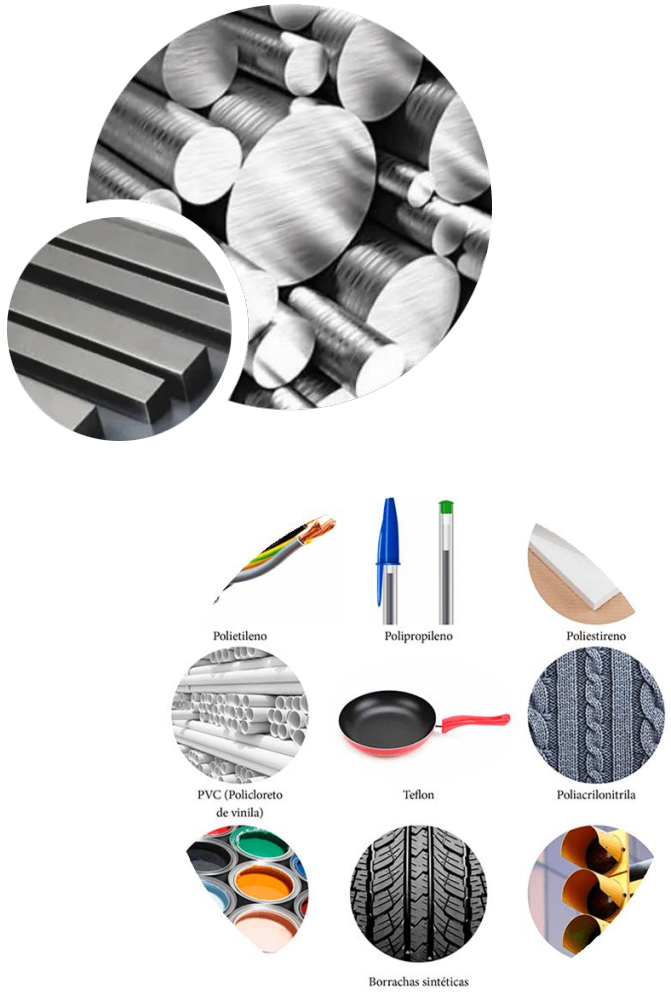
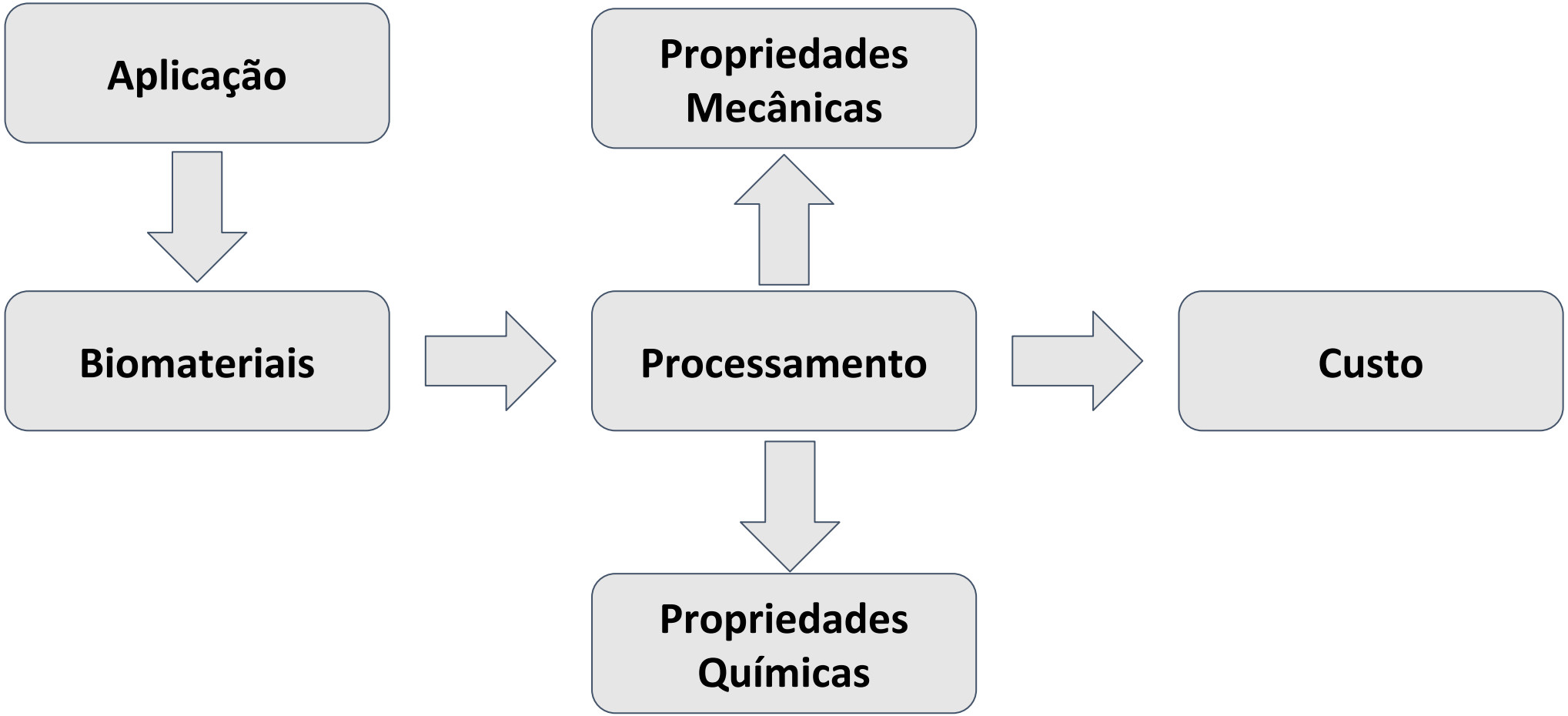


Figura 2 - Exemplos dos tipos de materiais: Metálicos, poliméricos, cerâmicos e compósitos.

Problemática



Problemática

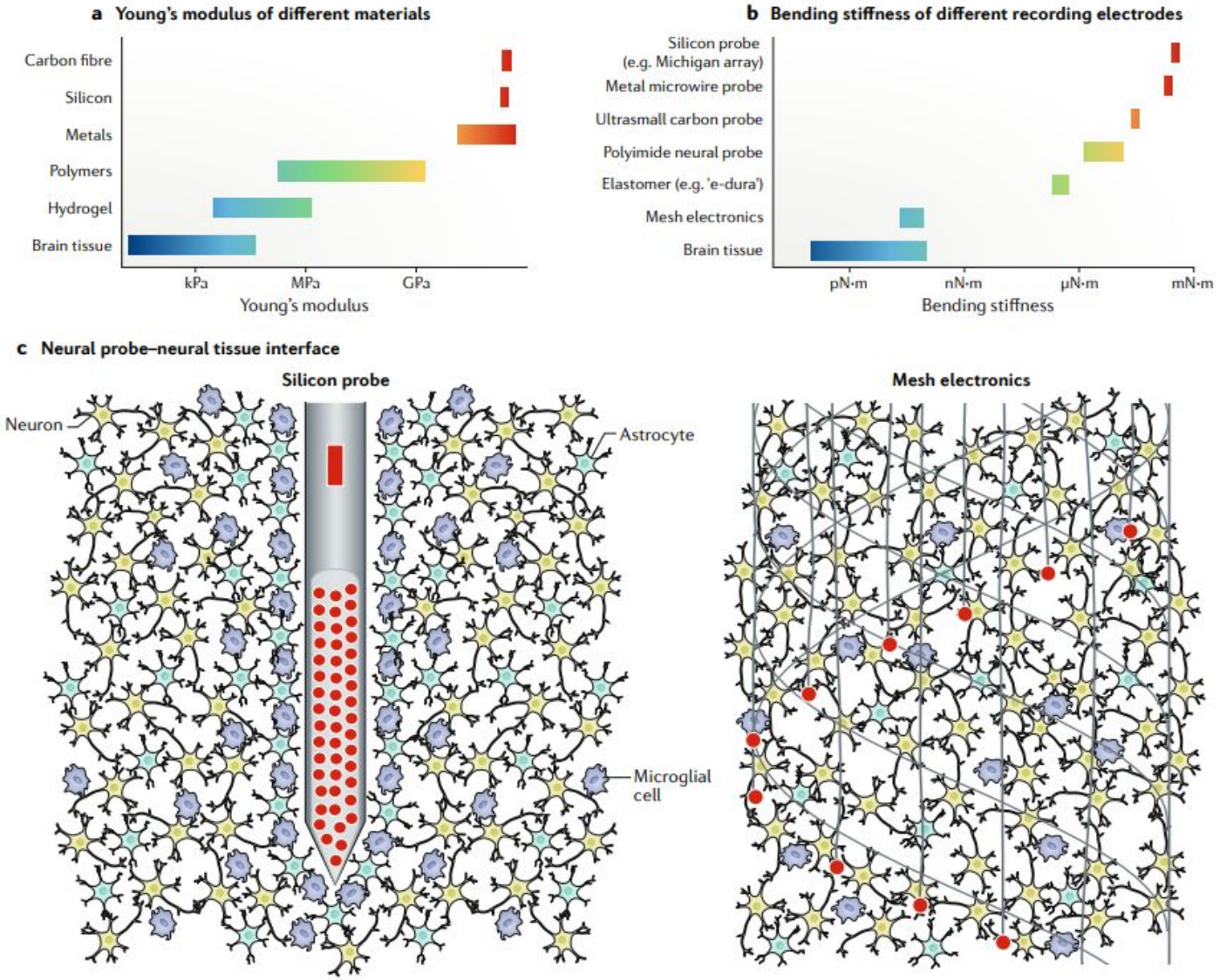
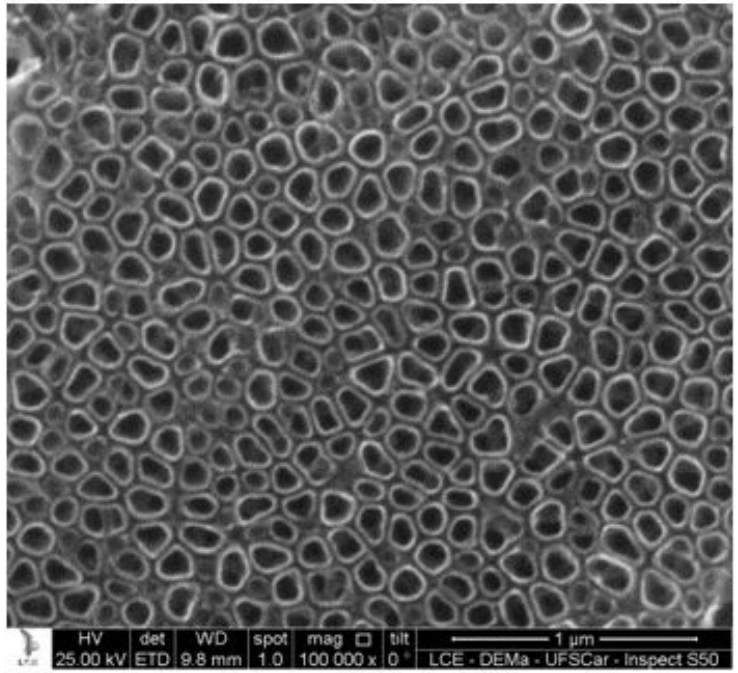
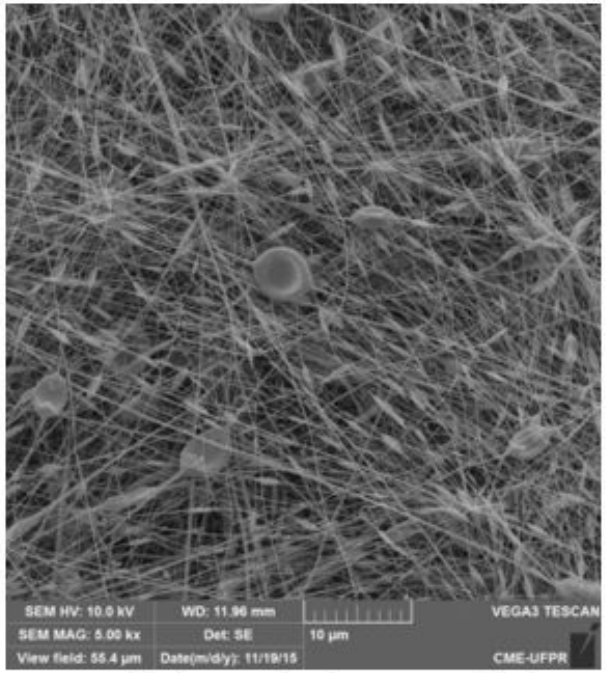


Figura 3 - a) Módulo de Young de diferentes materiais comparados ao tecido cerebral; b) Rigidez a Flexão de diferentes eletrodos. c)Interface de sonda neural-tecido neurol. Fonte: HONG 2019.

Problemática



Micrografia da película de dióxido de titânio crescida sobre a liga Ti6Al4V, em anodização potenciostática: 25 V por 1,5 h. (ROSSI, M.)



Micrografia da superfície do aço inoxidável ISO 5832-9 após deposição do revestimento de PMMA via eletrospinning (CAMARGO, E.)

Fonte: http://www.demec.ufpr.br/portal/gbio/tratamentos-superficiais/

Modificação da superfície

- **Anodização potenciostática**
- **Eletrospinning**
- **PECVD (Plasma Enhanced Chemical Vapor Deposition)**
- **Jateamento**

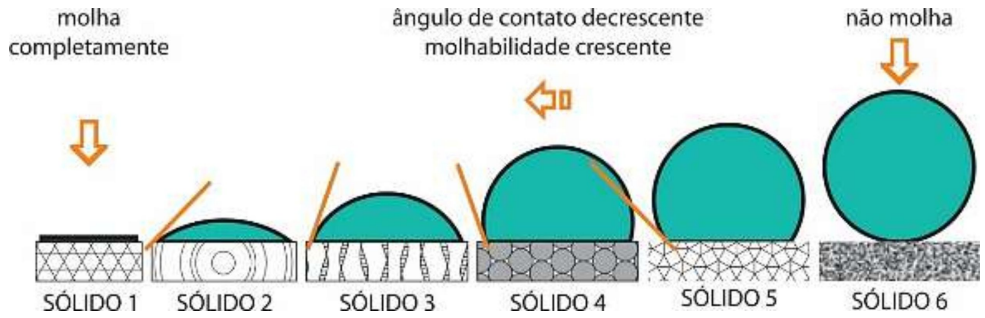
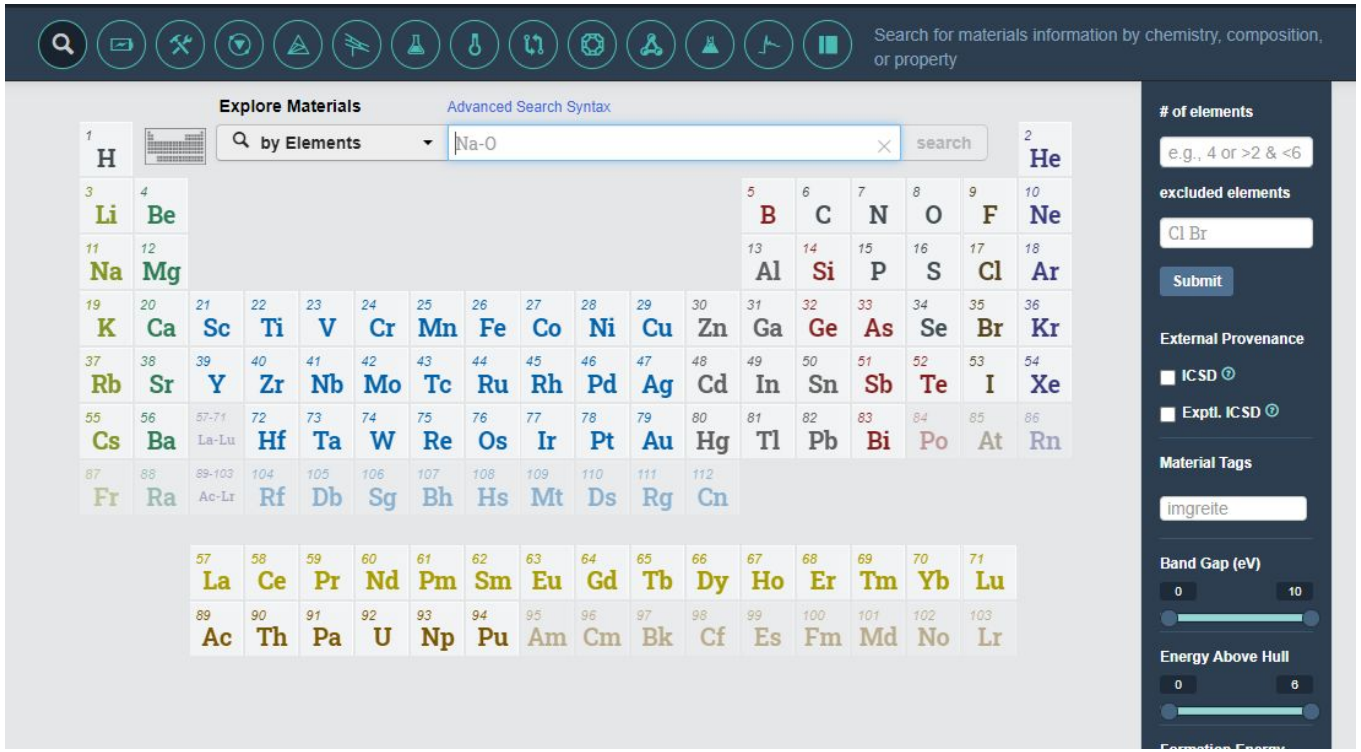
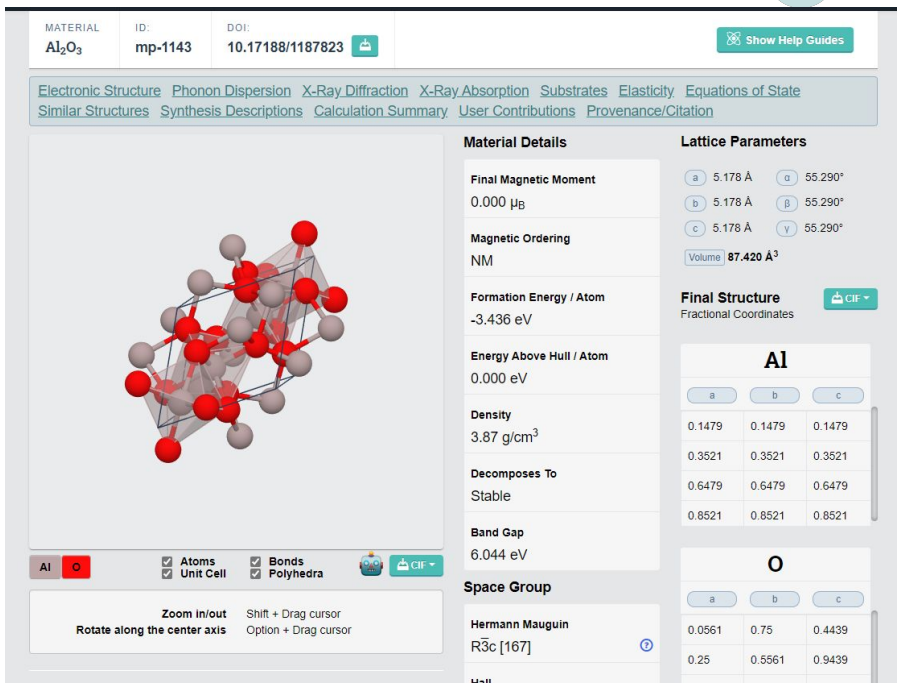


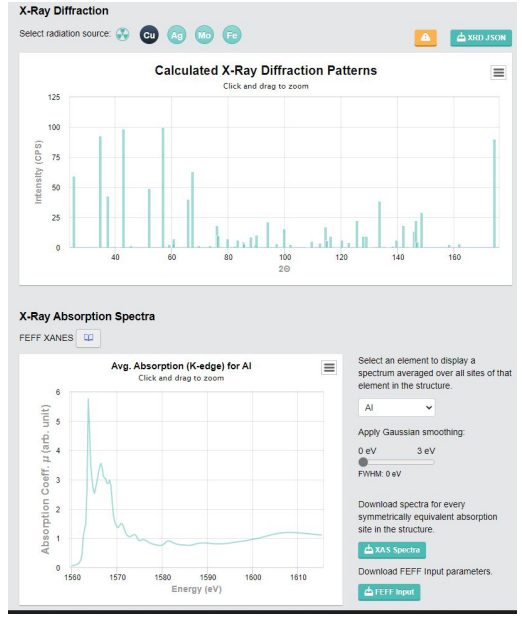
Figura x - Diferentes ângulos de contatos para 6 sólidos com superfícies distintas.
Fonte: DAPPER 2013

Ferramentas Utilizadas

Materials Project - Disponibiliza dados de milhares de materiais.







Fonte: https://materialsproject.org/

Ferramentas Utilizadas

Pymatgen.org

https://pymatgen.org/index.html

pymatgen
2020.9.14

Search docs

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- API Docs

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Edit on GitHub

pymatgen

Introduction

Testing - main passing | Testing - analysis passing | downloads 88k total | coverage 81%

Pymatgen (Python Materials Genomics) is a robust, open-source Python library for materials analysis. These are some of the main features:

1. Highly flexible classes for the representation of Element, Site, Molecule, Structure objects.
2. Extensive input/output support, including support for VASP (http://cms.mpi.univie.ac.at/vasp/), ABINIT (http://www.abinit.org/), CIF, Gaussian, XYZ, and many other file formats.
3. Powerful analysis tools, including generation of phase diagrams, Pourbaix diagrams, diffusion analyses, reactions, etc.
4. Electronic structure analyses, such as density of states and band structure.
5. Integration with the Materials Project REST API, Crystallography Open Database and other external data sources.

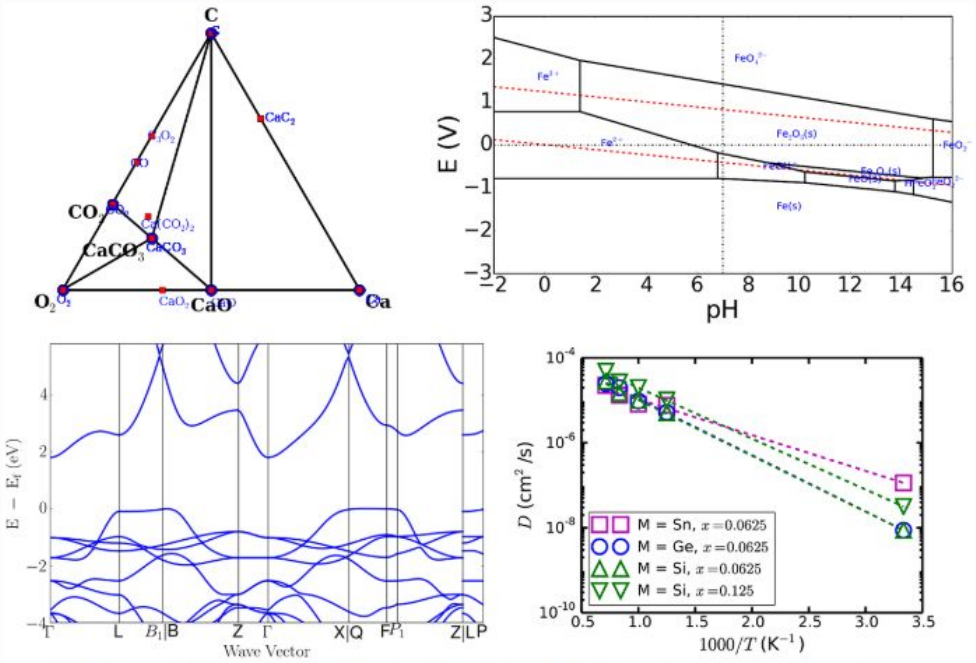
As of 2020, pymatgen only supports Python 3 and above.

Pymatgen is free to use. However, we also welcome your help to improve this library by making your own contributions. These contributions can be in the form of additional tools or modules you develop, or feature requests and bug reports. The following are resources for pymatgen:

Matgenie & Examples

The Materials Virtual Lab has developed a matgenie web app which demonstrates some of the basic functionality of pymatgen, as well as a matgenb repository of Jupyter notebooks for common and advanced use cases. We have deprecated the pymatgen examples page in favor of this more sustainable approach going forward. One of the ways you can contribute is to fork the matgenb repo and add your own examples.

Below are a quick look at some of the graphical output possible.



Top: (left) Phase and (right) Pourbaix diagram from the Materials API. Bottom left: Calculated bandstructure plot using pymatgen's parsing and plotting utilities. Bottom right: Arrhenius plot using pymatgen's DiffusionAnalyzer.

Fonte: https://pymatgen.org/index.html

Código

Referências

- JOSHI, Rajendra P. et al. Machine learning the voltage of electrode materials in metal-ion batteries. **ACS applied materials & interfaces**, v. 11, n. 20, p. 18494-18503, 2019.
- HONG, Guosong; LIEBER, Charles M. Novel electrode technologies for neural recordings. **Nature Reviews Neuroscience**, v. 20, n. 6, p. 330-345, 2019.
- REZENDE, Maria Cristina Rosifini Rosifini Alves et al. O papel da adsorção de proteínas na osseointegração. **ARCHIVES OF HEALTH INVESTIGATION**, v. 4, n. 3, 2015.
- A. Jain*, S.P. Ong*, G. Hautier, W. Chen, W.D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, K.A. Persson *(*=equal contributions)* **The Materials Project: A materials genome approach to accelerating materials innovation** APL Materials, 2013, 1(1), 011002.
- Pymatgen.org - Link: https://pymatgen.org/index.html

Obrigado!

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