

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
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- Problemática
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Artigo Base

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

Rajendra P. Joshi,^{†,‡} Jesse Eickholt,[‡] Liling Li,[‡] Marco Fornari,[†] Veronica
Barone,^{*,†} and Juan E. Peralta[†]

[†]*Department of Physics and Science of Advanced Materials Program, Central Michigan
University, Mount Pleasant, MI, 48859, USA*

[‡]*Department of Computer Science, Central Michigan University, Mount Pleasant, MI,
48859, USA*

E-mail: v.barone@cmich.edu

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

Crystal lattice type

Space group

An example input:

For an intercalation reaction: $0.5\text{Mg} + \text{Mg}_{0.5}\text{VO}_3 = \text{MgVO}_3$

High ion concentration: MgVO_3

Low ion concentration: $\text{Mg}_{0.5}\text{VO}_3$

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: MgCaNi_4

Low ion concentration: $\text{Mg}_{0.5}\text{CaNi}_4$

Fraction of metal-ion: 0.2

Type of metal-ion: Mg

Crystal lattice type: hexagonal

Space group: 194

[Submit another job.](#)

Introdução

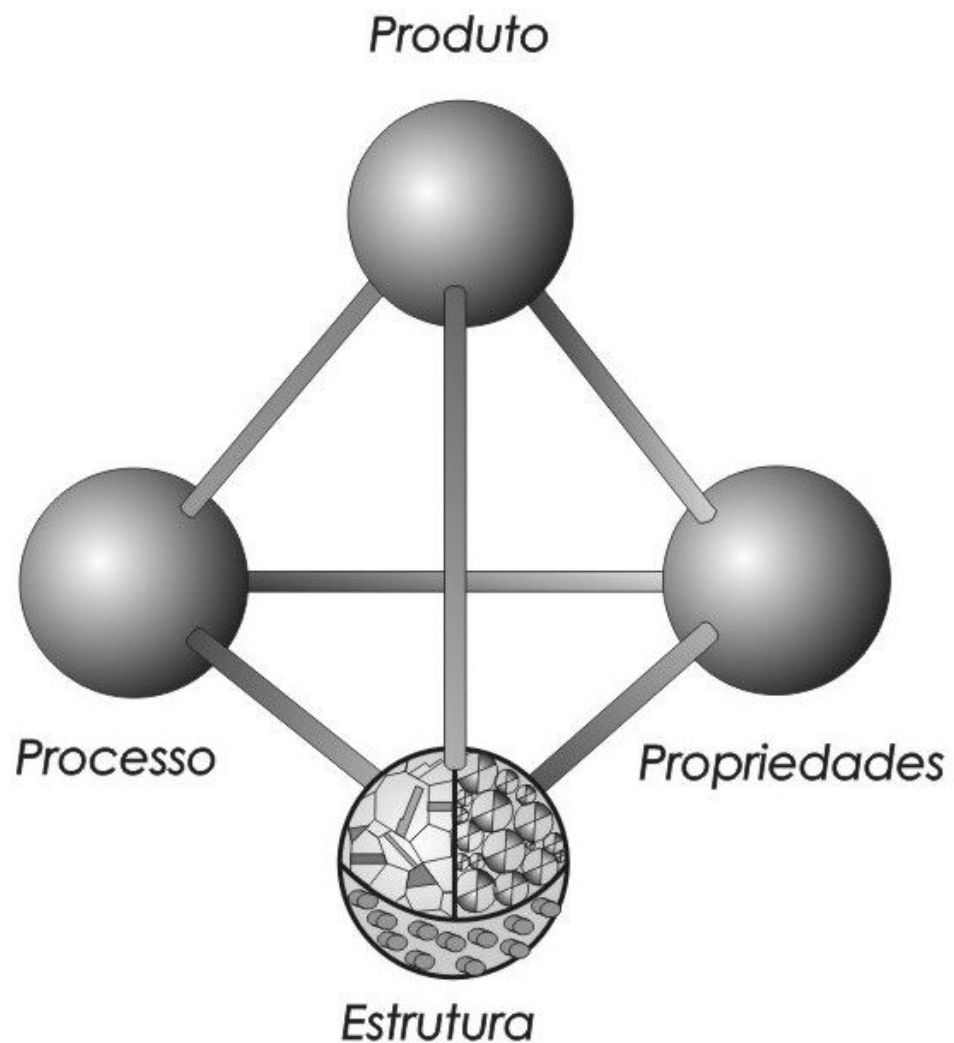


Figura 1 - Tetraedro de Ciência dos Materiais.
Fonte: Callister 8ªed.

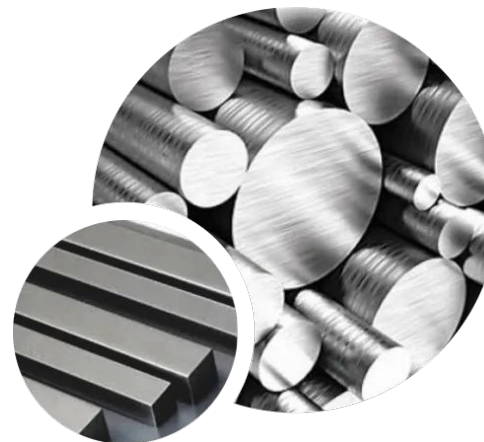
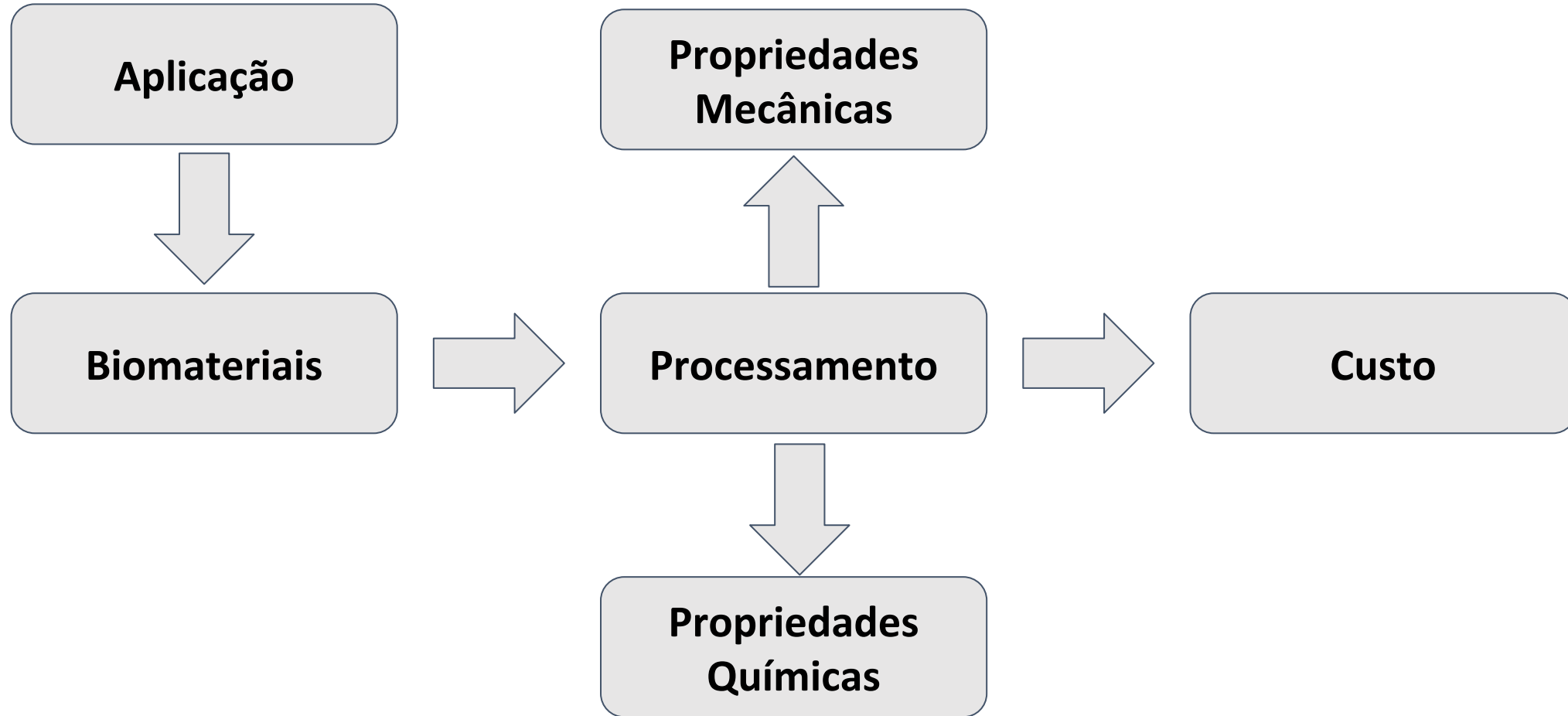


Figura 2 - Exemplos dos tipos de materiais:
Metálicos, poliméricos, cerâmicos e
compósitos.

Problemática



Problemática

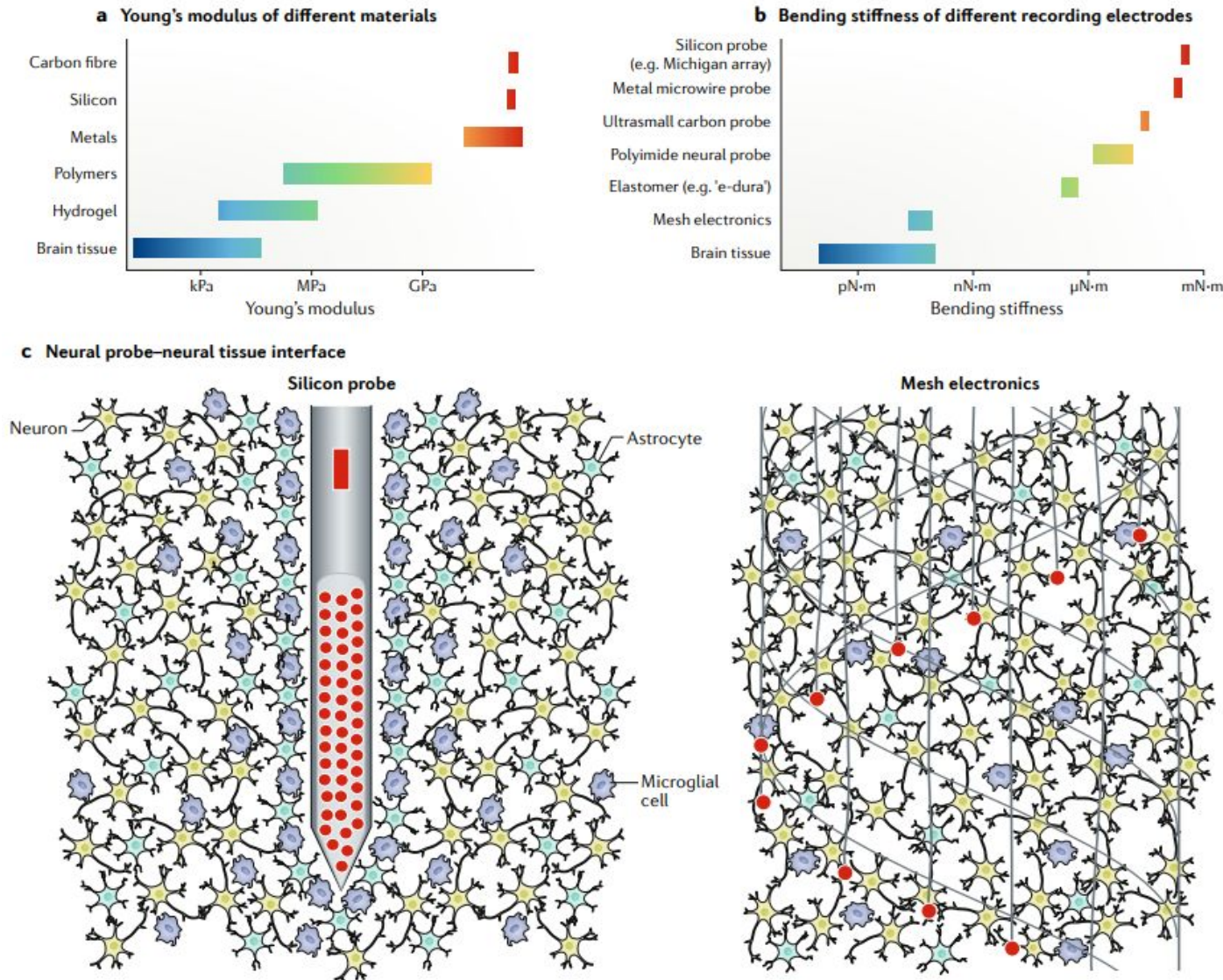
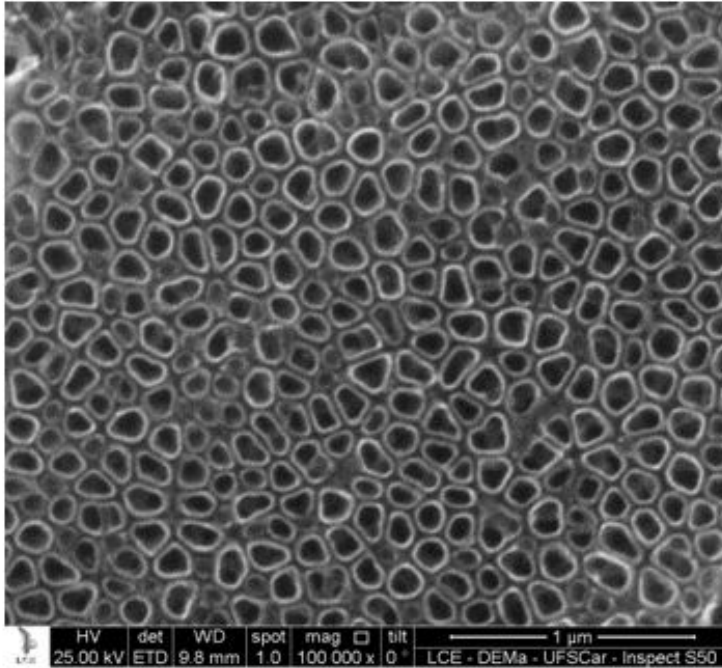
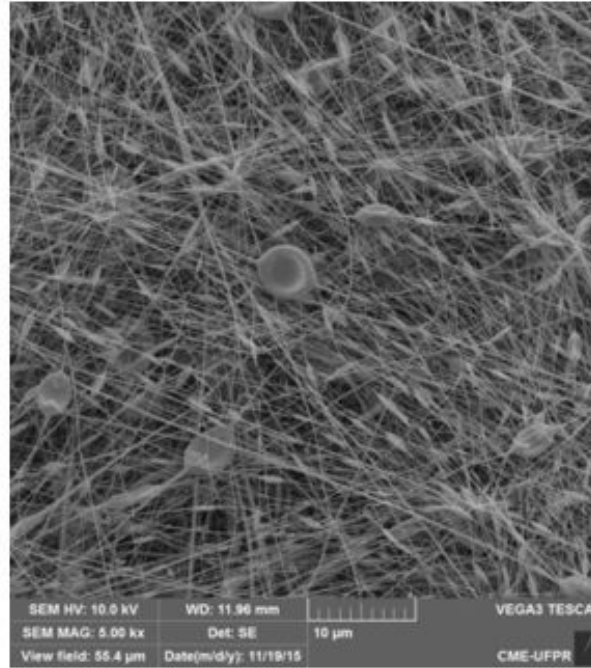


Figura 3 - a) Módulo de Young de diferentes materiais comparados ao tecido cerebral; b) Rigidez a Flexão de diferentes eletrodos. c) Interface de sonda neural-tecido neurol. Fonte: HONG 2019.

Problemática



Micrografia da película de dióxido de titânio crescida sobre a liga Ti6Al4V, em anodização potencioestática: 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.)

Modificação da superfície

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

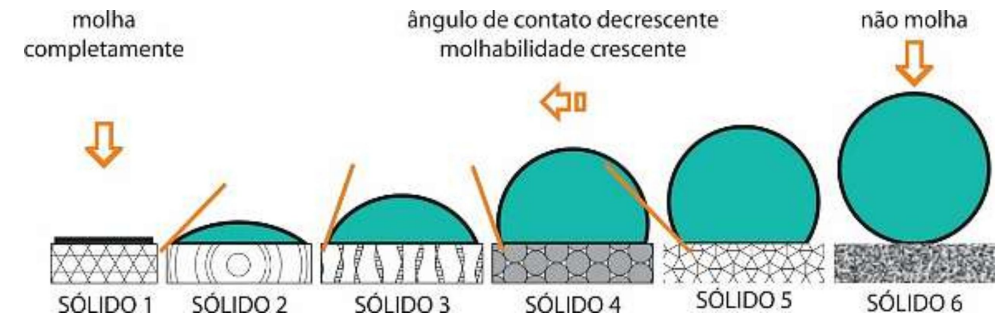


Figura x - Diferentes ângulos de contatos para 6 sólidos com superfícies distintas.

Fonte: DAPPER 2013

Ferramentas Utilizadas

Materials Project - Disponibiliza dados de milhares de materiais.

Search for materials information by chemistry, composition, or property

Explore Materials [Advanced Search Syntax](#)

by Elements search

1	H	2	He
3	Li	4	Be
11	Na	12	Mg
19	K	20	Ca
37	Rb	38	Sr
55	Cs	56	Ba
87	Fr	88	Ra
21	Sc	22	Ti
39	Y	40	Zr
57-71	La-Lu	72	Hf
89-103	Ac-Lr	104	Rf
23	V	24	Cr
41	Nb	42	Mo
73	Ta	74	W
105	Db	106	Sg
25	Mn	26	Fe
43	Tc	44	Ru
75	Re	76	Os
107	Bh	108	Hs
27	Co	28	Ni
45	Rh	46	Pd
77	Ir	78	Pt
109	Mt	110	Ds
29	Cu	30	Zn
47	Ag	48	Cd
79	Au	80	Hg
111	Rg	112	Cn
31	Al	32	Si
49	In	50	Sn
81	Tl	82	Pb
113	Nh	114	Fl
33	P	34	S
51	Sb	52	Te
83	Bi	84	Po
115	Mc	116	Lv
35	Br	36	Kr
53	I	54	Xe
85	At	86	Rn
61	Pm	62	Sm
89	Ac	90	Th
91	Pa	92	U
93	Np	94	Pu
95	Am	96	Cm
97	Bk	98	Cf
99	Es	100	Fm
101	Md	102	No
103	Lr	104	Uu

of elements
e.g., 4 or >2 & <6

excluded elements
Cl Br

Submit

External Provenance
☐ ICSD ☐ Exptl. ICSD

Material Tags
imgreite

Band Gap (eV)
0 10

Energy Above Hull
0 6

Formation Energy

Fonte: <https://materialsproject.org/>

MATERIAL: Al_2O_3 ID: mp-1143 DOI: 10.17188/1187823

Show Help Guides

Electronic Structure Phonon Dispersion X-Ray Diffraction X-Ray Absorption Substrates Elasticity Equations of State
Similar Structures Synthesis Descriptions Calculation Summary User Contributions Provenance/Citation

Material Details

Final Magnetic Moment
0.000 μ_B

Magnetic Ordering
NM

Formation Energy / Atom
-3.436 eV

Energy Above Hull / Atom
0.000 eV

Density
3.87 g/cm³

Decomposes To
Stable

Band Gap
6.044 eV

Lattice Parameters

a 5.178 Å b 5.178 Å c 5.178 Å

Volume 87.420 Å³

Final Structure
Fractional Coordinates

Al

a	b	c
0.1479	0.1479	0.1479
0.3521	0.3521	0.3521
0.6479	0.6479	0.6479
0.8521	0.8521	0.8521

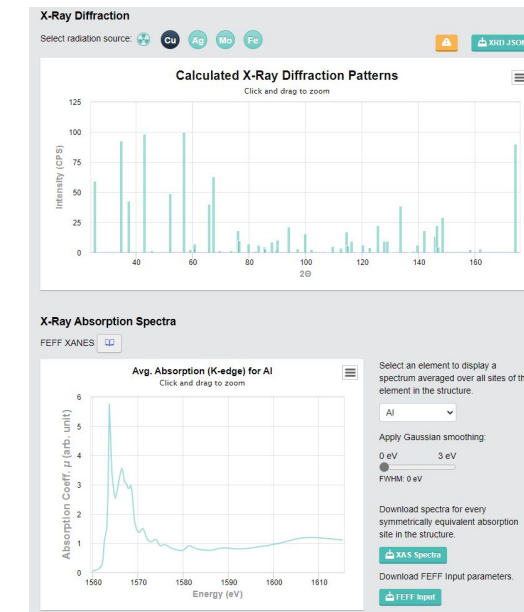
O

a	b	c
0.0561	0.75	0.4439
0.25	0.5561	0.9439

Space Group
Hermann Mauguin
R $\bar{3}c$ [167]

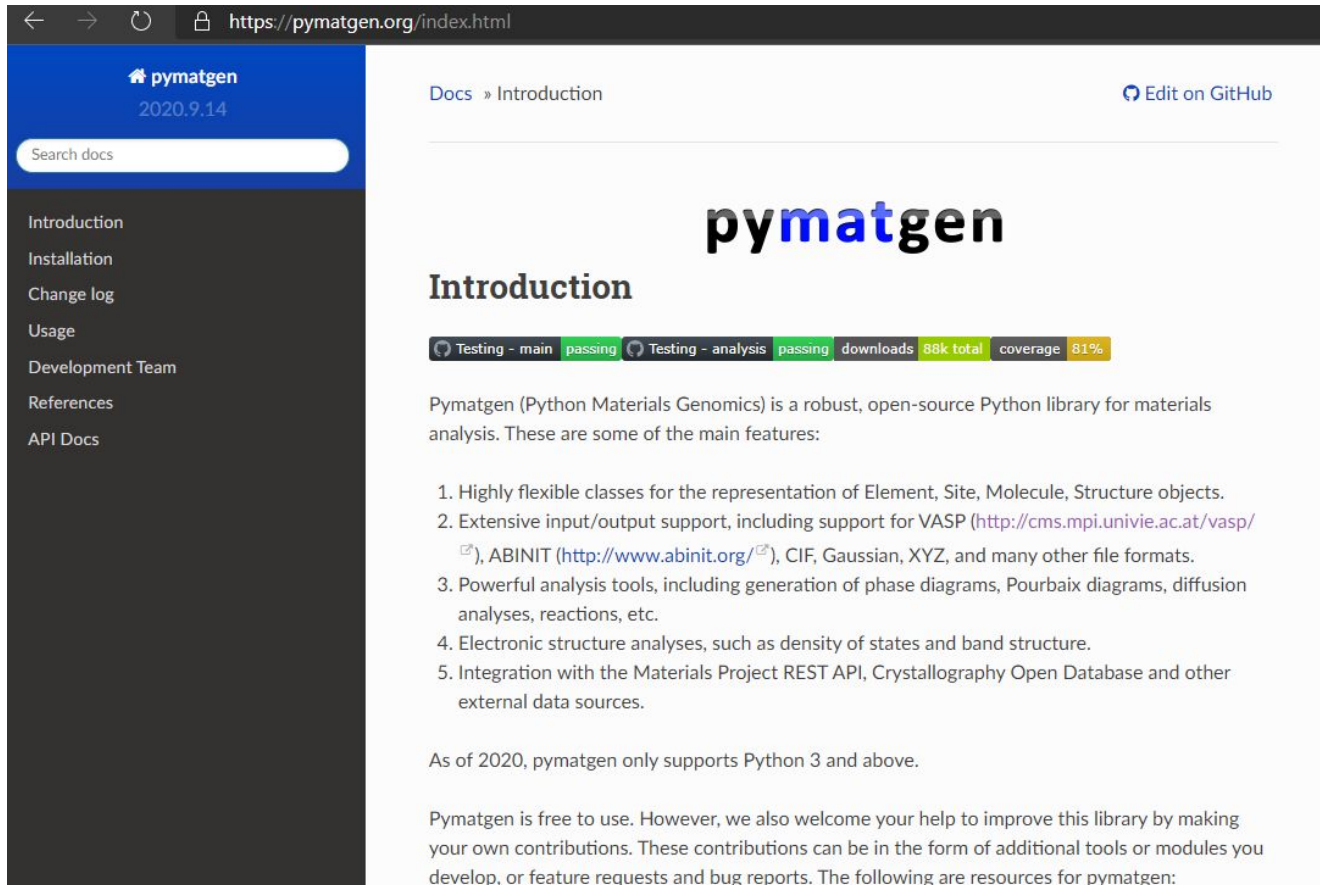
Zoom in/out Rotate along the center axis Shift + Drag cursor Option + Drag cursor

Atoms Unit Cell Bonds Polyhedra CIF



Ferramentas Utilizadas

Pymatgen.org

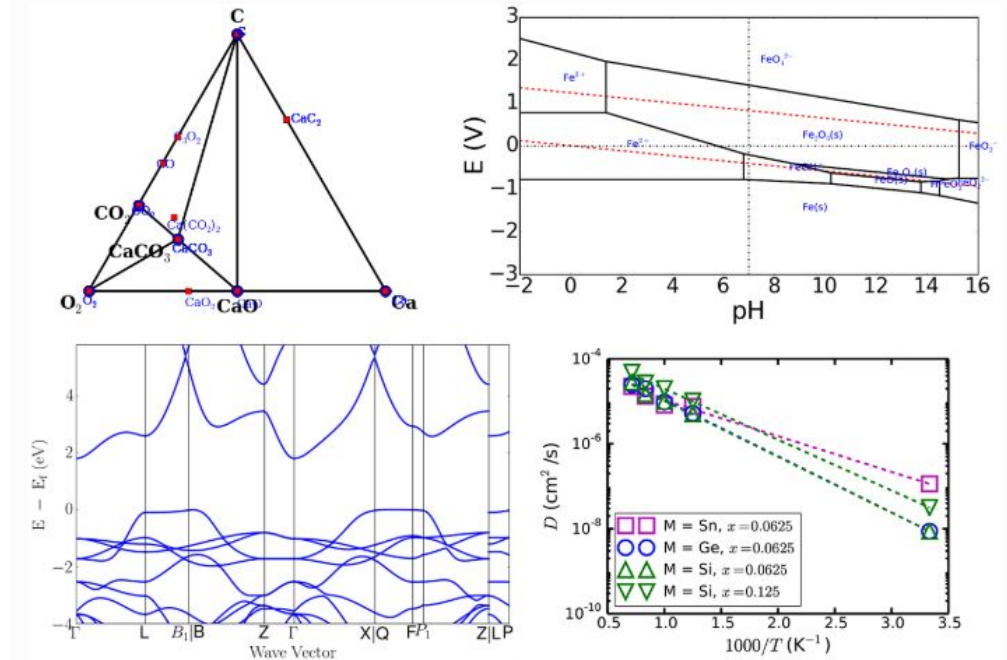


The screenshot shows the pymatgen.org website. The header includes the pymatgen logo and the date 2020.9.14. A search bar is present. The left sidebar lists navigation links: Introduction, Installation, Change log, Usage, Development Team, References, and API Docs. The main content area is titled 'pymatgen Introduction' and features a status bar indicating 'Testing - main passing', 'Testing - analysis passing', 'downloads 88k total', and 'coverage 81%'. The text describes pymatgen as a robust, open-source Python library for materials analysis. A list of five main features is provided: 1. Highly flexible classes for the representation of Element, Site, Molecule, Structure objects. 2. Extensive input/output support, including support for VASP, ABINIT, 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. At the bottom, it states that as of 2020, pymatgen only supports Python 3 and above, and welcomes contributions to improve the library.

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.

Código

Referências

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- 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!

E-mail: gilberto.filho@edu.isd.org.br

 institutosantosdumont.org.br

 contato@isd.org.br

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