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THE COMPUTATIONAL SCIENCE AND
ENGINEERING SOCIAL NETWORK

Gabriele Mogni
24th June 2019

SOCIAL MEDIA GROUPS: EFFECTIVE AND FAST MESSAGE DELIVERY TO LARGE AUDIENCES



1. SEMINARS / WEBINARS

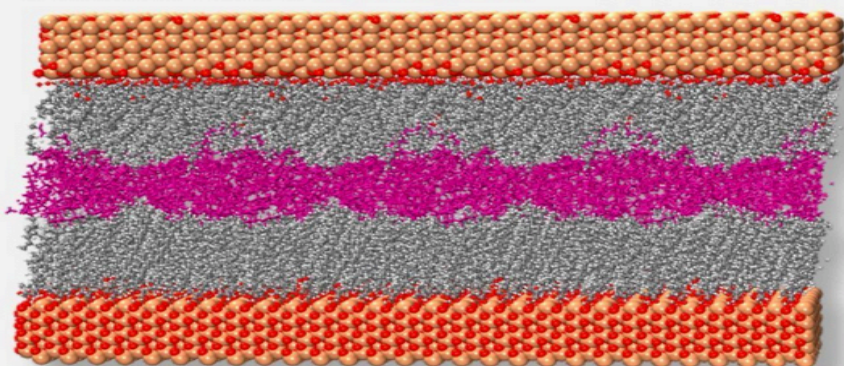


Xenophon Krokidis • 1st
Founder & Managing Director at Scienomics
9mo

...

SCIENOMICS WEBINAR: Sept. 27, 2018. Simulation of Lubricants and Refrigerants with MAPS. [#materials](#) [#lubrication](#) [#maps](#) [#materialsresearch](#) [#computationalchemistry](#) ...see more

SCIENOMICS WEBINAR



September 27, 2018: EU/Asia: 10 am CET- USA: 11 am PST
Predicting Properties and Behavior of Lubricants
and Refrigerants using MAPS

This webinar is dedicated to demonstrating how materials simulations and thermodynamic modeling can predict with MAPS technology rheological behavior, friction properties, solubility or phase equilibrium at high pressure. The typical workflow to generate results from molecular modeling involves the steps **BUILD > SIMULATE > ANALYZE** which can all be performed with SCIENOMICS' multiscale simulation platform, MAPS. Applications will include:

- phase equilibrium and solubility of a hydrofluoroolefin (HFO) refrigerant
- lubricant viscosity and friction behavior of a multi-component system

Anyone interested in lubricant and refrigerant systems will benefit from this free webinar and Q&A session. We will be pleased to have you with us!

MAPS
build • simulate • analyze

SCIENOMICS
delivering science

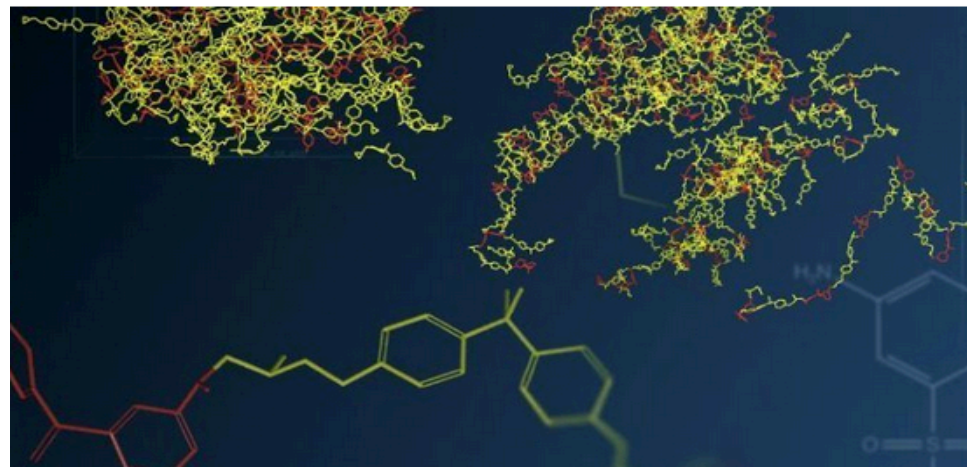


Thomas Mustard Ph.D. • 1st
Associate Principal Materials Scientist at Schrödinger, Inc.
1mo

...

What can Schrödinger do for your research and development?

Join our Materials Science Seminar week (May 7-10) and get to know, how Simulations and ML/AI could help finding novel solutions for polymers, organic electronics, energy storage, thin film processes, catalysis and complex formulations.



Current

[schrodinger.com](https://www.schrodinger.com)

1



Like



Comment

2. CONFERENCES / WORKSHOPS

 **Xenophon Krokidis** • 1st
Founder & Managing Director at Scienomics
10mo

SCIMEETING2018 - CONFERENCE ON MATERIALS SCIENCE SIMULATIONS IN INDUSTRY

SCIMEETING2018 - Oct. 30 - Nov. 1 2018 - Pittsburgh, PA - USA

Registration: <https://lnkd.in/dvsEdYY>

SCIMEETING is recognized as the meeting place of industrial innovation and multiscale simulations technology for Materials Science and Engineering. Atomistic, molecular, and mesoscale simulations as well as thermodynamic models and statistical models and predictions will be covered in this framework.

The conference will cover applications from several industrial areas including chemicals, personal & home care, oil & gas, materials, auto & aerospace, microtechnology, and pharmaceuticals.

Join us and participate in discussions with scientists from world-leading industries and Scienomics. We will be glad to have you with us!
hashtag#engineers hashtag#materials hashtag#simulations
hashtag#simulationsoftware hashtag#materialsscience
hashtag#materialsresearch hashtag#computationalchemistry
hashtag#computationalmodeling


<http://www.scienomics.com/scimeeting-usa-2018/>




SCIMEETING
OCT. 30-NOV. 2, 2018
Pittsburgh, USA

Simulations for Product and Process Design






SciMeeting-USA-2018
scienomics.com

 **Computational Science and Engineering Social Network**
Published by Gabriele Moggi [?] • 20 May •



Writing reproducible workflows using AiiDA



May 21st-24th, 2019, Lausanne

AiiDA is 😊 feeling excited.
20 May •

Getting ready for the #AiiDA tutorial starting tomorrow at Ecole polytechnique fédérale de Lausanne (EPFL), with over 50 participants expected, 4 invited speakers, 10 instructors, ... Stay tuned for updates on the event! #NCCR_MARVEL #MaX_CoE #swissuniversities #Psik #H2020intersect

226 People reached **11** Engagements Boost Unavailable

  You, Ramdayal Rana, Raju Mandal and 7 others

3. SUMMER SCHOOLS



Svitlana Iljenko • 2nd
CEO at MSI, Materials Science International GmbH
6mo

...

Early Bird Registration Deadline is coming soon- 20.12.2018.
3rd MSIT Winter School on Materials Chemistry, 3-6 March, 2019.
We are happy to inform you that the Programme of the MSIT Winter School and the MSIT Annual Seminar is online.

<https://lnkd.in/db7QiGg>

The topics of the Winter School will be linked link by considering a single binary system, with the students ultimately performing a full thermodynamic optimisation in Module "Computational Materials Thermodynamics". The intention is to introduce participants to the system through the experimental data that will be discussed in the other modules. In the 'practical' sessions the data relevant to the selected system will be discussed in more detail.

PLEASE NOTE: the early-bird deadline is in 2 days only – 20.12.2018. Use your chance to register at a reduced fee!

<https://lnkd.in/dYAthVU>

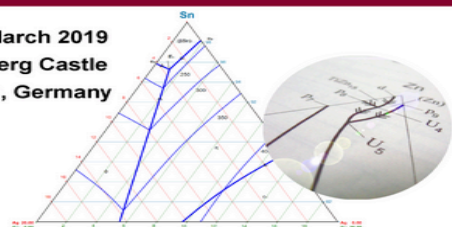
#chemistry #materials #computation #thermodynamics

Early Bird Registration deadline is 20.12.2018!



Winter School

3 - 6 March 2019
Ringberg Castle
Kreuth, Germany



Organised by

Dr. Günter Effenberg / MSI,
Materials Science International
GmbH, Germany

Prof. Andrew Watson / Coventry
University, United Kingdom

Dr. Frank Stein, Dr. Martin Palm /
Max-Planck-Institut für
Eisenforschung GmbH, Germany

3rd MSIT Winter School on Materials Chemistry

The Programme is online

www.msiport.com

Like Comment



Daniele Varsano • 2nd
Research Scientist at Consiglio Nazionale delle Ricerche, Institute of Nan...
2mo

...

The Quantum ESPRESSO Foundation and the EU MaX Centre for Materials at the exascale, in association with the Jožef Stefan Institute, are proud to announce a one-week event entitled:

"Summer School on Advanced Materials and Molecular Modelling with QUANTUM ESPRESSO"

Jožef Stefan Institute (Ljubljana, Slovenia), September 16–20, 2019

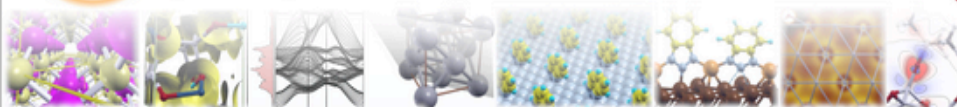
Further info available at <http://qe2019.ijs.si/>



QUANTUM ESPRESSO

Summer School on Advanced Materials and Molecular Modelling

September 16–20, 2019
Ljubljana, Slovenia



8

Like Comment

4. JOB OFFERS



Katherine H. • 2nd
Materials Design, Inc.
4mo

NOW HIRING A SUPPORT SCIENTIST <https://lnkd.in/grDq7FK> Materials Design is excited to announce a search for a new colleague who will enhance our Support team and provide solutions to our growing user community. The formal advertisement is available on <https://lnkd.in/grDq7FK>. We are looking for applicants with a PhD in computational materials science or related fields to support our users applying MedeA to solve their research problems and open new areas of exploration in the field of atomistic simulations. If you know of a candidate with such expertise, please encourage them to apply. They are welcome to submit a cover letter and resume with a selected list of publications to recruiting@materialsdesign.com #physics, #computationalmaterialsscience #modeler #chemistry, #materials #science, #modeling, #simulations, #VASP, #LAMMPS, #GIBBS, #MOPAC, #Gaussian #scientist #hiring #hiringnow, #hiring

Materials Design Inc | Careers

materialsdesign.com

The MedeA software package developed by Materials Design is the leading environment for the atomist...

5



Like



Comment



Kristen Williams • 2nd
Senior Materials Engineer at Boeing
1mo



Kristen Williams • 2nd
Senior Materials Engineer at Boeing
1mo • Edited

My group is looking for an engineering supervisor to manage employees performing technical activities predominantly in these areas: Surface Treatments and Finishes, Corrosion Modeling and Testing. ...see more



Materials Process & Physics First Line Manager in United States, Alabama, Huntsville

boeing.referrals.selectminds.com




Like




















Comment





5. POLLS AND SURVEYS



 **Gabriele Mogni** created a poll. Admin · 1 November 2017


The best overall ab-initio DFT software is.....



VASP Added by Gabriele Mogni	   +22
Quantum Espresso Added by Gabriele Mogni	   +17
gaussian Added by Niles Choudhary	   +8
SIESTA Added by Gabriele Mogni	   +3
Wien2k Added by Strange Attractor	   +3
6 more options...	


  Mecanica Cuantica Perú, Lei Yang and 5 others 7 comments 1 share



 Like  Comment  Share 


 **Jason Lawrence McAfee** Depends on the problem you want solved.
Like · Reply · 1y  3






↳  Gabriele Mogni replied · 1 reply

 **Mikael Kuisma** GPAW. Written in python, most readable source code, easy to use, basis sets, plane waves and real space grid, lots of extensions.
Like · Reply · 1y  3

↳  Manana Ko replied · 1 reply

 **Tymofii Nikolaienko** Why ORCA is not in the list????
Like · Reply · 1y  1

↳  Tymofii Nikolaienko replied · 2 replies

 Write a comment...    

6. NEW SOFTWARE RELEASES



Gabriele Mogni

Technical Consultant at European Materials Modelling Council
5mo

...



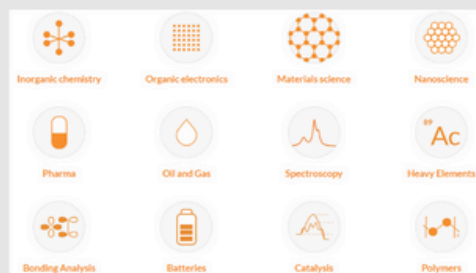
Software for Chemistry & Materials

733 followers
5mo

We hope 2019 is off to a flying start for you. As most of the SCM team is back in the office after a refreshing break, we're all ready to take on your **#compchem** challenges! We love to hear about your research and how we can make make computational chemistry work for you!

Post your research question or software development request in the comments below or go to our website: <https://lnkd.in/gWHyPXm>

Amsterdam Modeling Suite



Empowering researchers worldwide in many areas since the 1970s
Reach out to discuss, or just try for yourself!

1

Like Comment



Synopsys Simpleware Software • 2nd

From 3D images to models
6mo • Edited

...

Synopsys Simpleware O-2018.12 Out Now - Learn about the latest release

<http://bit.ly/2PtDNbp>



2

Like Comment

7. INTERESTING WEBSITES

Computational Science and Engineering Social Network
Published by Gabriele Moggi [?] · 19 May ·

Some useful resource for computational chemists 😊
<https://pubchem.ncbi.nlm.nih.gov/>

PubChem About Blog Submit Contact PubChem Periodic Table and Element pages Read More >

Explore Chemistry
Quickly find chemical information from authoritative sources

Try aspirin EGFR C9orf4 S7-27-2 C1=CC=C(C=C)C1C=O HCN=15/C3H4O(1-3)/24H1-243

Draw Structure Upload ID List Browse Data Periodic Table

98M Compounds 245M Substances 266M Bioactivities 30M Literature 3M Patents 671 Data Sources
See More Statistics > Explore Data Sources >

PUBCHEM.NCBI.NLM.NIH.GOV
PubChem
Search and explore chemical information in the world's largest freely...

873 **75**
People reached Engagements **Boost Post**

👍 Raju Mandal, Junichi Sugishita and 8 others 1 comment 8 shares

Computational Science and Engineering Social Network
shared a link to the group: **QUANTUM SERVER: COMPUTATIONAL SCIENCE AND ENGINEERING.**
Published by Gabriele Moggi [?] · 10 March ·

<https://www.physics.rutgers.edu/gbrv/>

PHYSICS.RUTGERS.EDU
GBRV pseudopotentials
Updated September 23, 2015 Version 1.5 now available. See below,...

191 **24**
People reached Engagements **Boost Unavailable**

👍 Nathan Caudill, Joao-carlos Das Neves Pereira and 11 others 1 share

8. VIDEOS



Computational Science and Engineering Social Network

Published by Gabriele Mogni [?] · 27 April · 🌐



Peter Koval shared a link to the group: Simune Atomistics.

27 April



YOUTUBE.COM

Scientists create first billion-atom biomolecular simulation

Researchers have created the largest simulation to date of an entire gene of DNA, a feat that...



163

People reached

17

Engagements

Boost Unavailable



Giuliano Xillo, Rudra Prakash and 10 others

1 share



Erik Feder · 2nd

Corporate Strategy and Communications at Fraunhofer IWM

2w

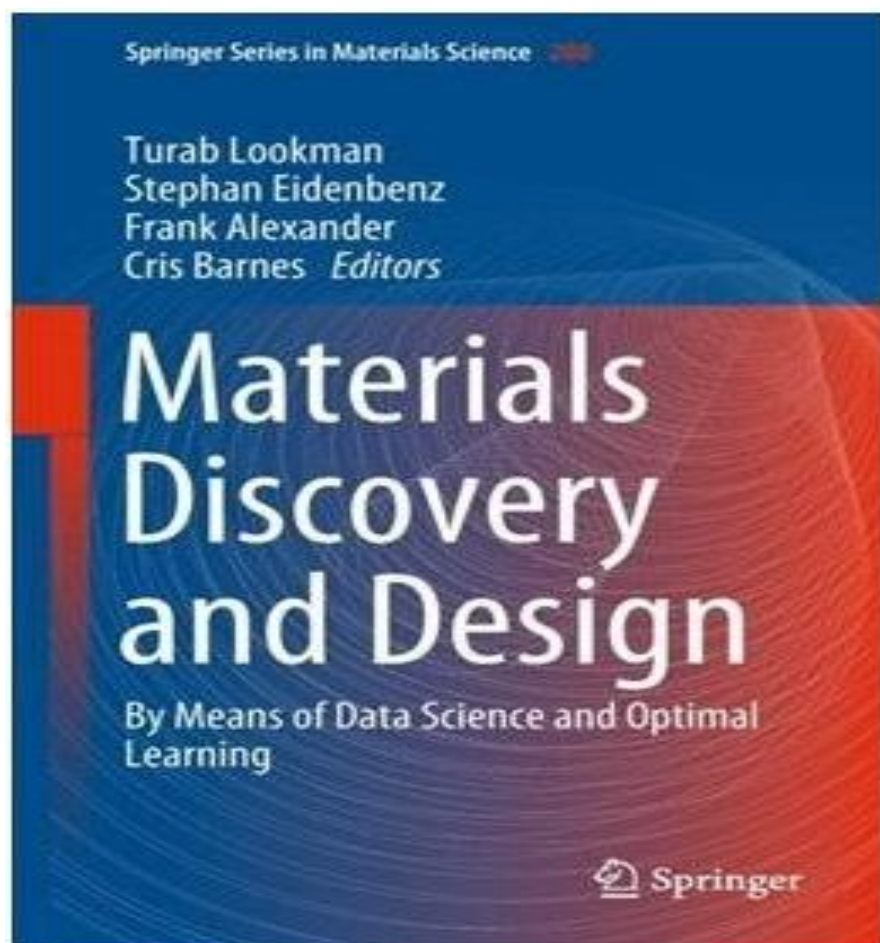



<https://lnkd.in/d9n5QrW> #materialsscience #materialtesting #validation #fracture



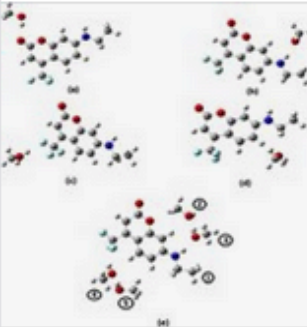
Material deformation, damage and crack formation, Dr. Michael Luke, Fr...
youtube.com

9. JOURNAL ARTICLES AND BOOKS



 **रक्षित मिश्र** shared a link.
19 March 2018



Hi everyone. I have just published an article in the journal "Computational and theoretical chemistry". The link of the journal is pasted below:









SCIENCEDIRECT.COM

Computational study of effect of solvents on vibrational spectra of coumarin 500






Optimized structure of coumarin 500 has been obtained in gas phase and in solvents like methanol, ethanol, dimethyl sulfoxide and CCl₄...

  El Wardano, Kacem Prince and 7 others 1 comment 1 share


 Like  Comment  Share 

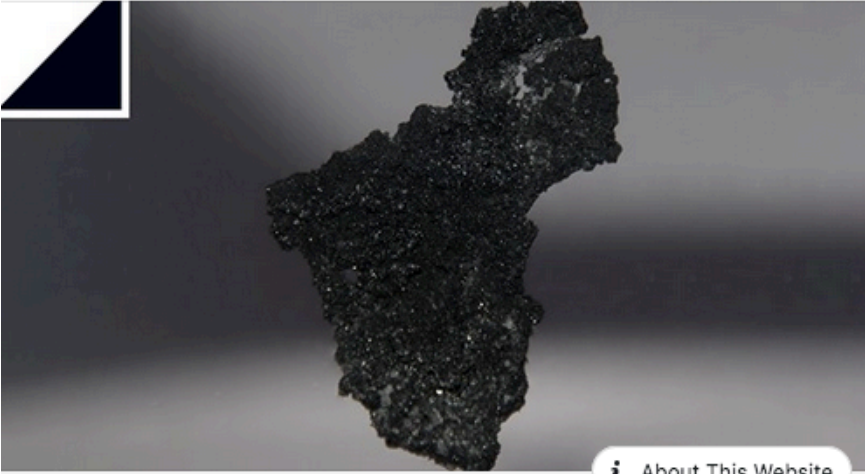
 **Saeed Azar** Congratulations  1

Like · Reply · 1y

 Write a comment...    

10. GENERAL NEWS AND ARTICLES

**Computational Science and Engineering Social Network**
Published by Gabriele Mogni [?] · 1 June at 12:10 · 🌐



[About This Website](#)




TECHNOLOGYREVIEW.COM

Sorry, graphene—borophene is the new wonder material that's got everyone excited


858
People reached


161
Engagements


Boost Post


 Dharmraj Saini, Ajay Jogna and 78 others


17 shares


 Like

 Comment

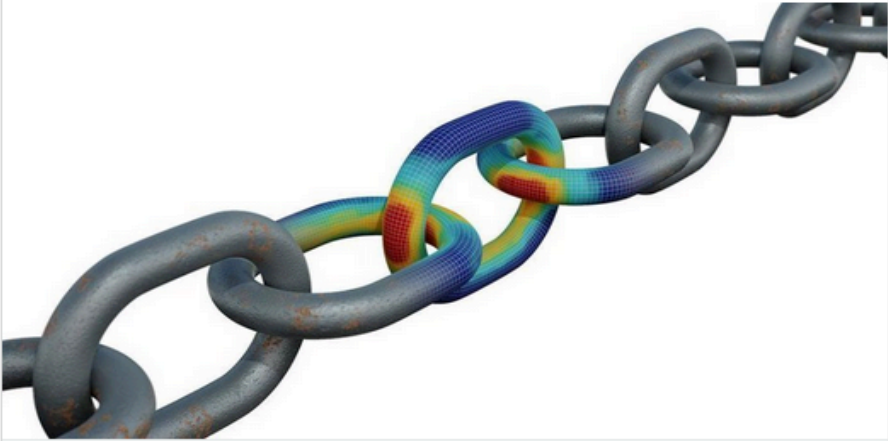
 Share




**Gabriele Mogni**
Technical Consultant at European Materials Modelling Council
1mo


**Mark Reisig** • 3rd+
Director of Product Marketing at Aras Corporation
1mo


This is an article I wrote on the democratization of Simulation and Analysis that appears in **Manufacturing.net**: <https://lnkd.in/emT7bHR> **#business** **#simulationsoftware** **#simulations** **#systemsengineering** **#plm**



The Democratization of Simulation and Analysis
manufacturing.net

 2

 Like

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EVEN MORE GENERAL NEWS AND ARTICLES

**Computational Science and Engineering Social Network**
Published by Gabriele Mogni [?] · 28 March · 🌐



python

[About This Website](#)

FOSSBYTES.COM | BY [MANISHA PRIYADARSHINI](#)
Python Is the Most Asked-About Language On Stack Overflow
According to a Global App Testing report, Python has overtaken...

759
People reached

106
Engagements

Boost Post

 Pallavi Warkhede, Michele Pavone and 70 others
6 shares

**Gabriele Mogni** shared a post.
Admin · 15 June at 12:22

**MIT Technology Review**
15 June at 08:21
[Like as your Page](#)

Code-breaking quantum computers are significantly closer to reality than anyone suspected.



TECHNOLOGYREVIEW.COM
How a quantum computer could break 2048-bit RSA encryption in 8 hours

2 shares

 Like

 Comment

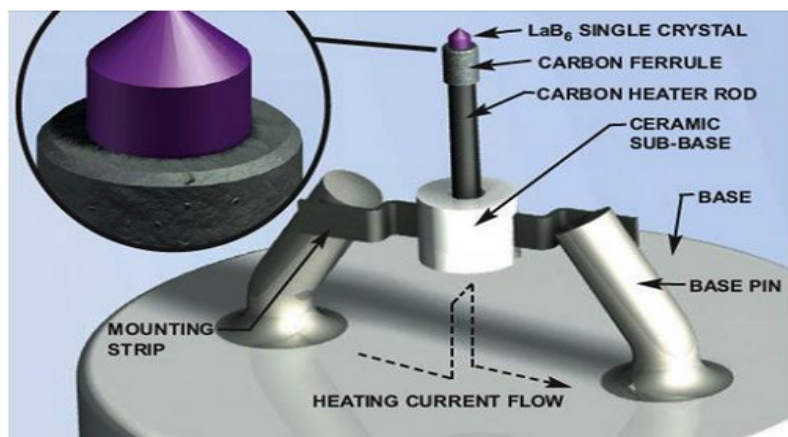
 Share



MATERIAL OF THE DAY BLOG SERIES

MATERIAL OF THE DAY: Lanthanum hexaboride

Lanthanum hexaboride (LaB_6 , also called lanthanum boride and LaB) is an inorganic chemical, a boride of lanthanum. It is a refractory ceramic material that has a melting point of 2210 °C, and is insoluble in water and hydrochloric acid. It has a low work function and one of the highest electron emissivities known, and is stable in vacuum. Stoichiometric samples are colored intense purple-violet, while boron-rich ones (above $\text{LaB}_{6.07}$) a... [See more](#)



1,349

People reached

137

Engagements

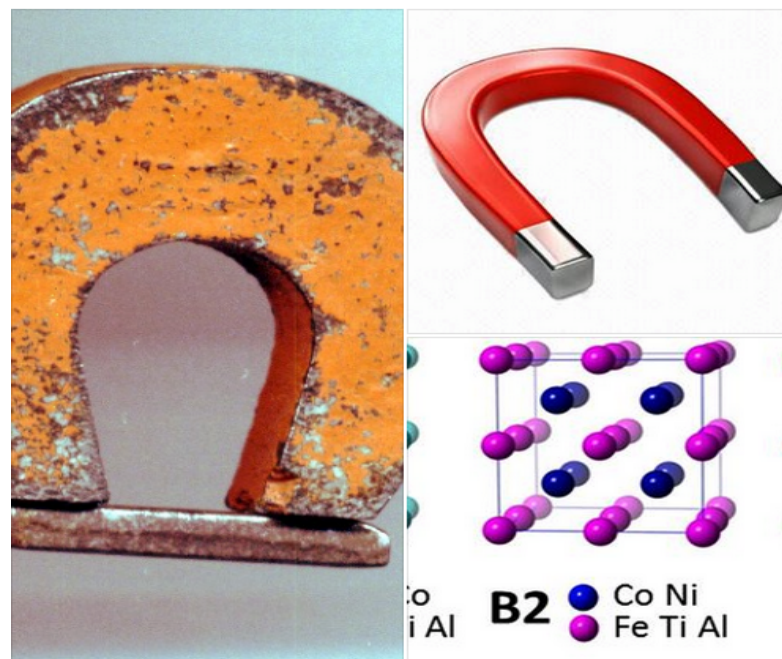
Boost Post

👍 🤖 Paardhasaradhi Kuppala, Ajay Jogna and 28 others

9 shares

Alnico is an acronym[1] referring to a family of iron alloys which in addition to iron are composed primarily of aluminium (Al), nickel (Ni) and cobalt (Co), hence al-ni-co. They also include copper, and sometimes titanium. Alnico alloys are ferromagnetic, with low coercivity-its resistance to loss of magnetism varies by grade from 630–1,880 oersteds (50–150 kA/m)[2]-and it is used to make permanent magnets. Before the development of rare-earth mag...

[Continue reading](#)



1,091

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93

Engagements

Boost Post

👍 Robert Blethen, Yasuo Matsushima and 22 others

10 shares