

**NOMAD**  
NOVEL MATERIALS DISCOVERY

## A Primer to NOMAD




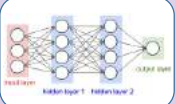
1) Open Science!  
2) Discovering Interpretable Patterns, Correlations, and Causality in Big Data of Materials

Introducing a New Research Paradigm

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## Introduction of New Paradigms to Materials Science and Engineering



### Knowledge in Materials Science and Engineering

<p><b>1<sup>st</sup> paradigm:</b> Empirical Science</p>   <p>Experiments</p>	<p><b>2<sup>nd</sup> paradigm:</b> Theoretical Science (Laws and Models)</p> $\Delta U = Q - W$ <p>Change in internal energy    Heat added to system    Work done by system</p> <p>Laws of classical mechanics, electrodynamics, thermodynamics, quantum mechanics</p>	<p><b>3<sup>rd</sup> paradigm:</b> Computational Science (Simulations)</p>  <p>Density-functional theory and beyond, molecular dynamics</p>	<p><b>4<sup>th</sup> paradigm:</b> Big-Data-Driven Science</p>  <p>Detection of patterns and anomalies in Big Data; machine learning, etc.</p>
1600	1950	2010	year

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NATURE | EDITORIAL  

# Empty rhetoric over data sharing slows science

**Governments, funders and scientific communities must move beyond lip-service and commit to data-sharing practices and platforms.**

12 June 2017

**nature** International weekly journal of science   [Advanced search](#)

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NATURE | EDITORIAL  

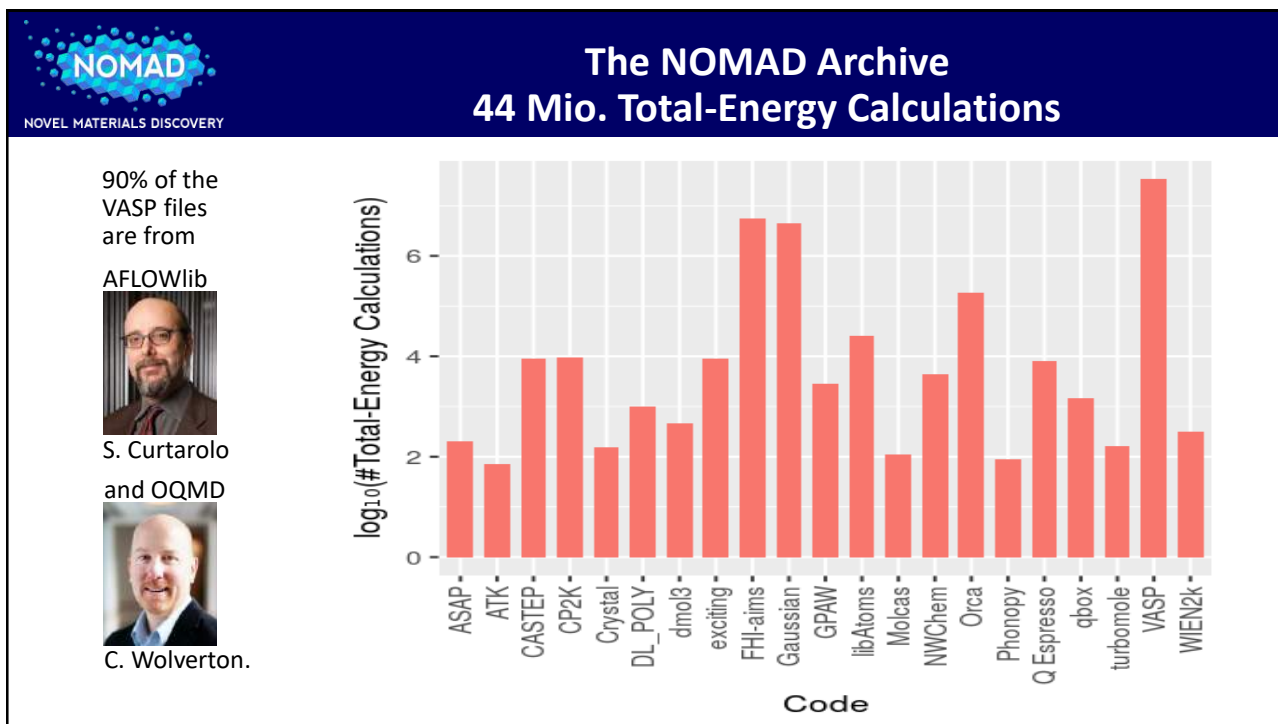
# Empty rhetoric over data sharing slows science

**Computational materials: Open data settled in materials theory**

**Claudia Draxl, Francesc Illas & Matthias Scheffler**

*Nature* **548**, 523 (31 August 2017) | doi:10.1038/548523d

Published online 30 August 2017



https://nomad-coe.eu

**NOMAD**  
The NOMAD Laboratory  
A European Centre of Excellence

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REPOSITORIES THE ARCHIVE ENCYCLOPEDIA BIG-DATA ANALYTICS ADVANCED GRAPHICS HPC INFRASTRUCTURE OUTREACH

**The Novel Materials Discovery (NOMAD) Laboratory** maintains the largest **Repository** for input and output files of all important computational materials science codes.

From its open-access data it builds several **Big-Data Services** helping to advance materials science and engineering.

[Watch a 3-minute summary on the NOMAD Laboratory CoE](#)

**NOMAD Scope and Overview**  
**Data is a crucial raw material of the 21st century.**

Surprisingly, extreme-scale aspects of Big-Data are very much under-explored in materials science and engineering, one reason being that 'towards

Recent Success Stories

Thermal-barrier coatings have driven the fuel-efficiency improvement in turbines over the last 30 years.



Heat conductivity (from low to high) is key for many technologies.

Events & Announcements  
Jun 1, 2017



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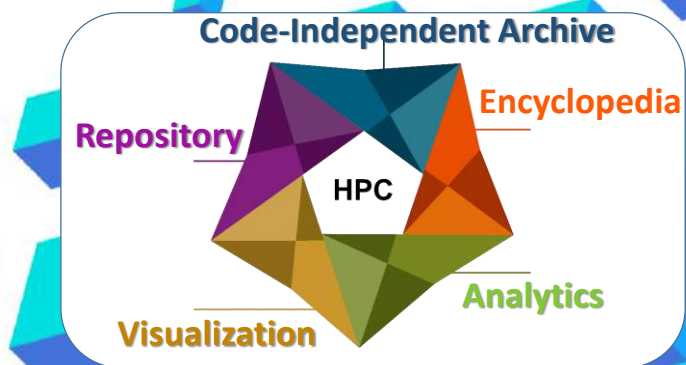
## The NOMAD Laboratory A European Centre of Excellence

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The NOMAD Repository accepts /requests in- and output files of all important codes. Currently, the NOMAD Repository contains **> 40 million** total-energy calculations.

30-40 important codes are used in computational materials science. The heterogeneity could hardly be worse.



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**NOMAD Repository**

Keeps data for at least 10 years  
Open access (if wanted with delay)  
Provides DOIs (make data citable)

<https://repository.nomad-coe.eu>  
also described at youtube.com

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**Code-Independent Archive**

**Conversion Layer**

**Repository**

**HPC**

**Encyclopedia**

**Analytics**

**Visualization**

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## The Big-Data Challenge

**(Big) Data of materials does not only provide direct information but the data is structured.**

**Volume** (amount of data),  
**Variety** (heterogeneity of form and meaning of data),  
**Velocity** at which data may change or new data arrive,  
**Veracity** (uncertainty of quality).

**A map of materials**

Thermal-barrier materials  
Photovoltaics  
Transparent metals  
Superconductors

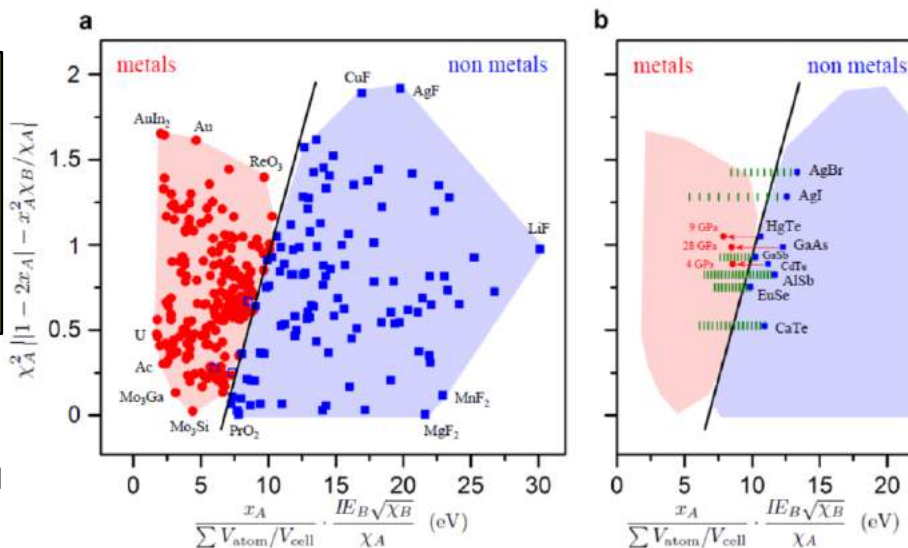
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## Classification of Materials in terms of Metal vs. Non-Metal

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The identified descriptors depend on properties of the **free atoms** and the **unit-cell volume**!

Runhai Ouyang,  
Stefano Curtarolo,  
Emre Ahmetcik,  
Matthias Scheffler, and  
Luca M. Ghiringhelli,  
to be published.



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## Significant Progress ... But Our Knowledge Is Still Close to Zero

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About **240,000** inorganic compounds have been synthesized so far.  
**Many more are possible.**

And what do we know?

Topological insulators 3D: 42, 2D: 7


Elastic constants: about 200 compounds

Dielectric constant  $\approx$  300-400













Heat conductance  $\approx$  200


Superconductors  $\approx$  1,000

*For almost every property we are well below 1% in coverage ....*














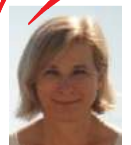
**The NOMAD Executive Team**

 <b>Matthias Scheffler</b> , FHI MPS, Berlin	 <b>Kristian Thygesen</b> Tech. U., Lyngby	 <b>Ciaran Clissmann</b> pintail Ltd. Dublin	 <b>Dieter Kranzlmüller</b> , LRZ Garching	 <b>Jose Maria Cela</b> , BSC, Barcelona	 <b>Alessandro De Vita</b> King's Col. London
 <b>Angel Rubio</b> MPI MPSD, Hamburg	 <b>Risto Nieminen</b> Aalto U. Helsinki	 <b>Kimmo Koski</b> CSC – IT Center Helsinki	 <b>Francesc Illas</b> U. of Barcelona	 <b>Stefan Heinzl</b> MPS Comp. & Data, Garching	 <b>Claudia Draxl</b> Humboldt U, Berlin
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**The NOMAD Executive Team**

**... and numerous highly motivated PhD students and postdocs!**

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## September 25-29 – A Typical Week in Berlin

**44<sup>th</sup> BERLIN MARATHON**







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## September 25-29 – A Typical Week in Berlin


*International Max Planck  
Research School*  
**Functional Interfaces  
in  
Physical Chemistry**  
Fall Block Course:  
Sept. 26 - Oct. 06, 2017



**Hybrid Inorganic/Organic  
Systems: HIOS Young Researcher  
Workshop 2017, Sept. 26-28**



**BDC**  
BERLIN BIG DATA CENTER  
Evaluation:  
Sept. 25, 26



**Future and Emerging Technologies**  
**HORIZON 2020**  
The EU Framework Programme  
for Research and Innovation  
**SMART** Speeding up **Materials** Data in **Real Time**  
Submission deadline: Sept. 26, 5:00 pm





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## Summary and Outlook

<https://nomad-coe.eu>

**Thanks!**

**Enjoy the workshop**

**Work hard**

**PLEASE tell us how  
we can/should  
improve**

