Mathematical modeling in the modern materials science

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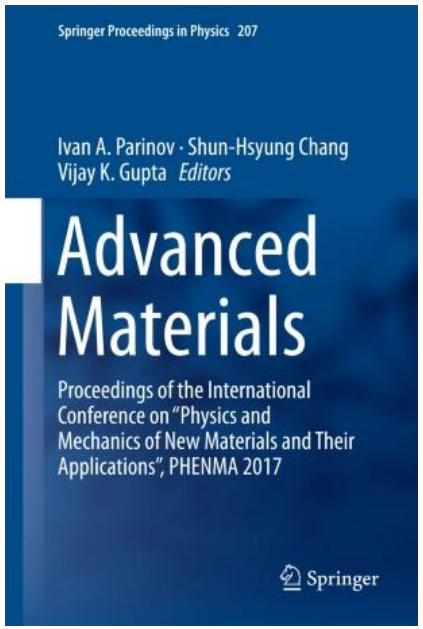
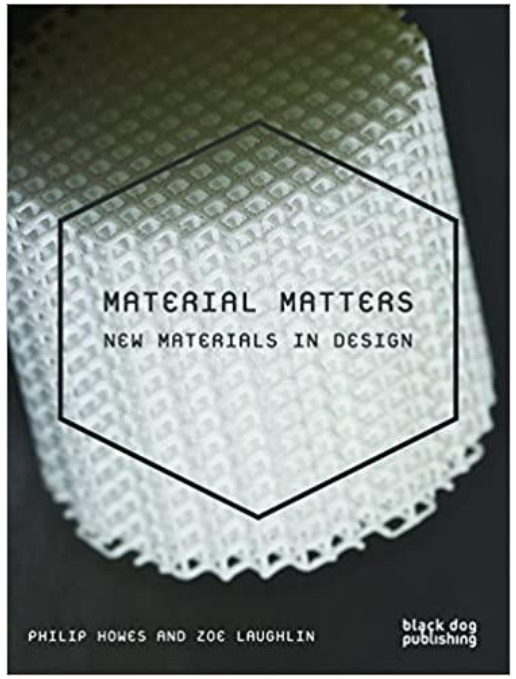
2021

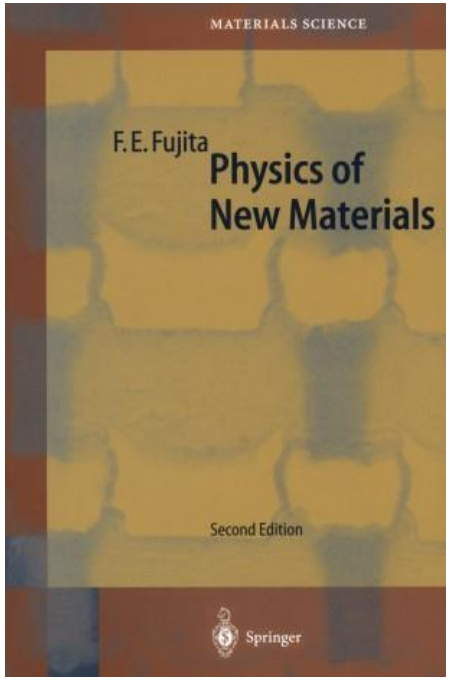
ver. 1.0

Materials science

Materials science is a syncretic discipline hybridizing metallurgy, ceramics, solid-state physics, and chemistry. It is the first example of a new academic discipline emerging by fusion rather than fission (source: *Wikipedia*).







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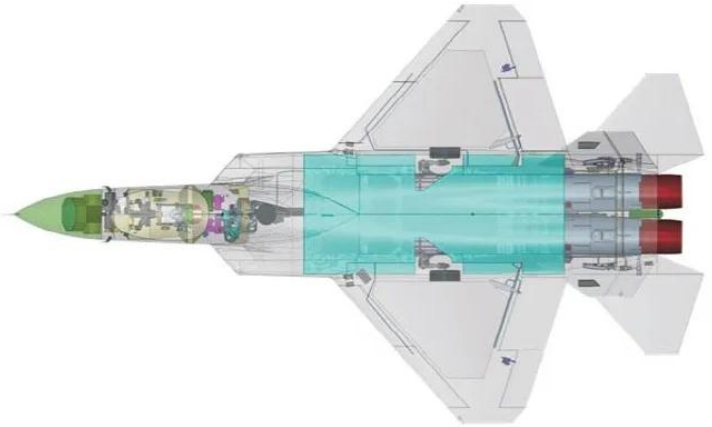
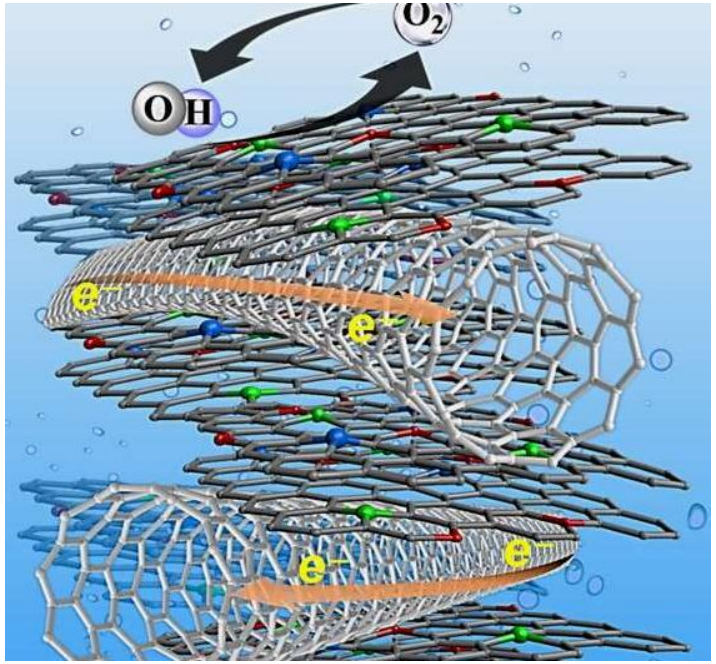
New materials change our lives





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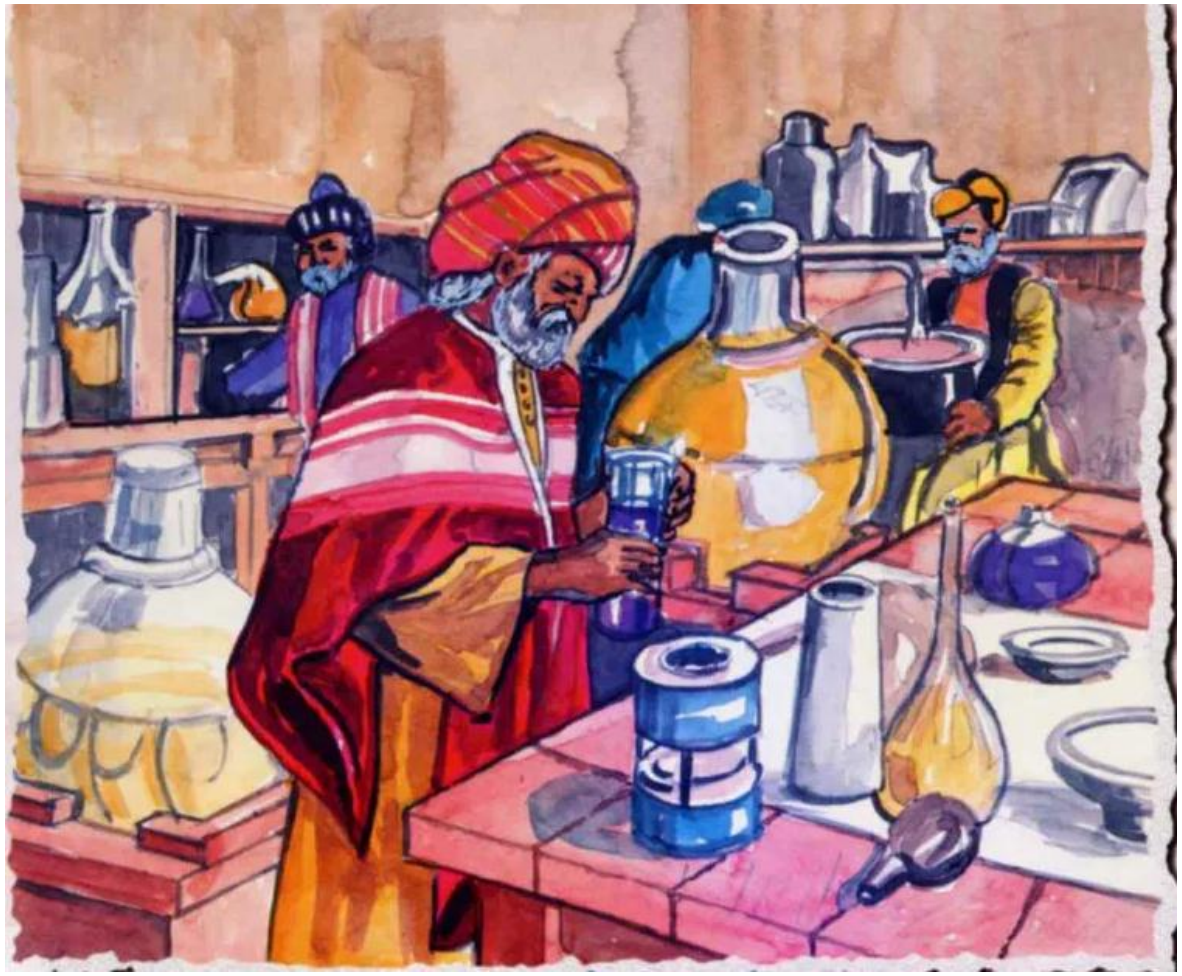
Traditional (experimental) materials science



The Venus of Dolní Věstonice, ceramic statuette dated to 29,000–25,000 BCE. The oldest known ceramic articles in the world.

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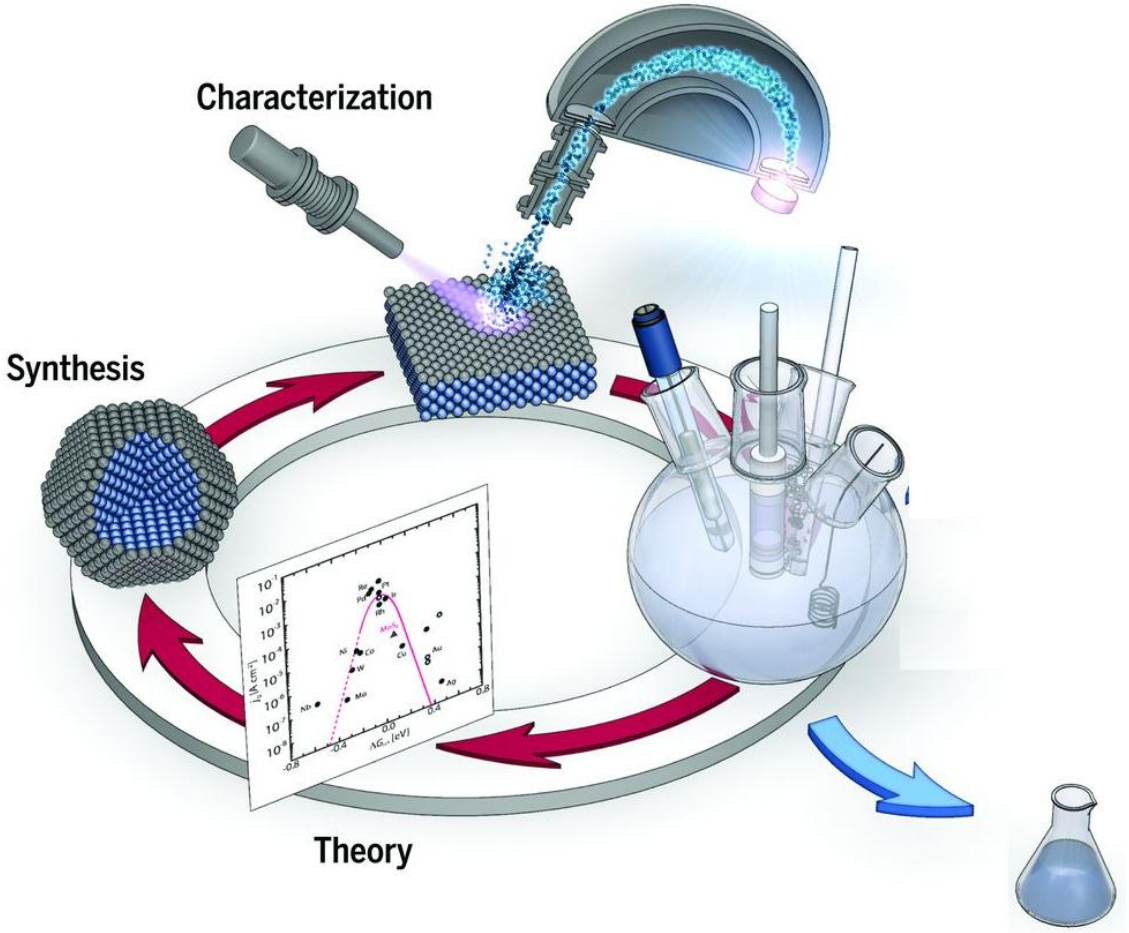
Theoretical materials science



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Theoretical materials science. DFT

(1)

This paper deals with the ground state of an interacting electron gas in an external potential $v(\mathbf{r})$. It is proved that there exists a universal functional of the density, $F[n(\mathbf{r})]$, independent of $v(\mathbf{r})$, such that the expression $E \equiv \int v(\mathbf{r}) n(\mathbf{r}) d\mathbf{r} + F[n(\mathbf{r})]$ has as its minimum value the correct ground-state energy associated with $v(\mathbf{r})$.

(2)

$$E = \int v(\mathbf{r}) n(\mathbf{r})\, d\mathbf{r} + \frac{1}{2} \int\int \frac{n(\mathbf{r}) n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\, d\mathbf{r}\, d\mathbf{r}' + G[n], \qquad (2.1)$$

where $n(\mathbf{r})$ is the density and $G[n]$ is a universal functional of the density. This expression, furthermore, is a minimum for the correct density function $n(\mathbf{r})$. In this

DFT: 1964-1965 гг.

Nobel Prize: 1998
W.Kohn
J. Pople

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DFT calculations

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cp2k

a computational tool for solid state chemistry and physics
CRYSTAL

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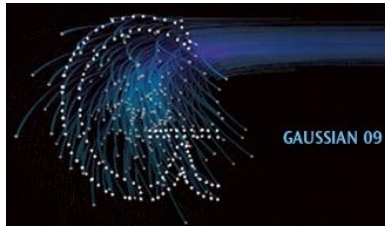

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$$c_{ijkl} = \frac{\partial^2 E}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}}$$

- Матрица упругих жесткостей C_{ij}
- Модуль Юнга E (T)
- Модуль сдвига G (T)
- Модуль объемного сжатия K (T)
- Коэффициент Пуассона (❍)
- G/K – мера хрупкости/эластичности вещества

$$\begin{pmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{pmatrix}$$

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{41} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{bmatrix}$$

- Фононные спектры
- Теплоемкость Cp, Cv
- Коэффициент теплового расширения α(P,T)
- Оценка процессов окисления
- Зонная структура
- Магнитная восприимчивость

$$\varepsilon_{ij}(\omega) E_j(\omega, \mathbf{s}) = \tilde{n}^2(\omega)$$
$$\{E_i(\omega, \mathbf{s}) - s_i s_j E_j(\omega, \mathbf{s})\}$$

- Тензор диэлектрической проницаемости
- Показатель преломления, коэффициент поглощения, отражательная способность

$$\begin{pmatrix} \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon \end{pmatrix} \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{pmatrix}$$

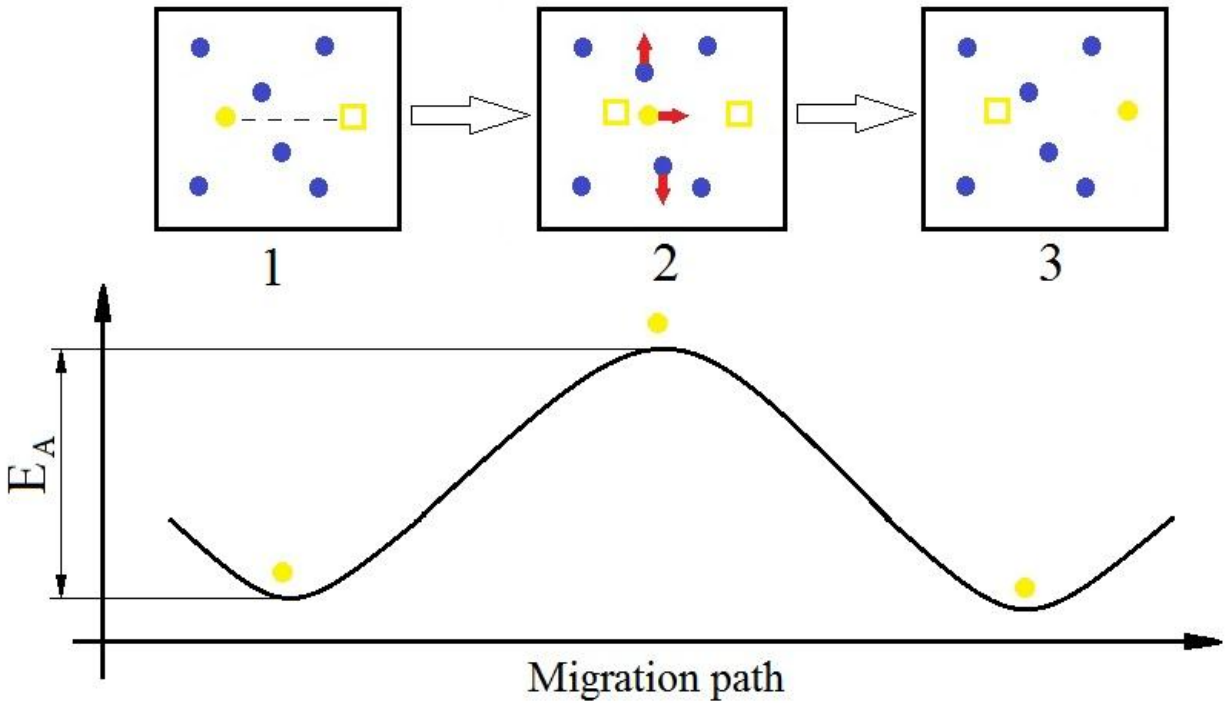
- ИК и Рамановские спектры

$$p_{uv} = \frac{\partial \Delta \varepsilon_u^{-1}}{\partial \eta_v}$$

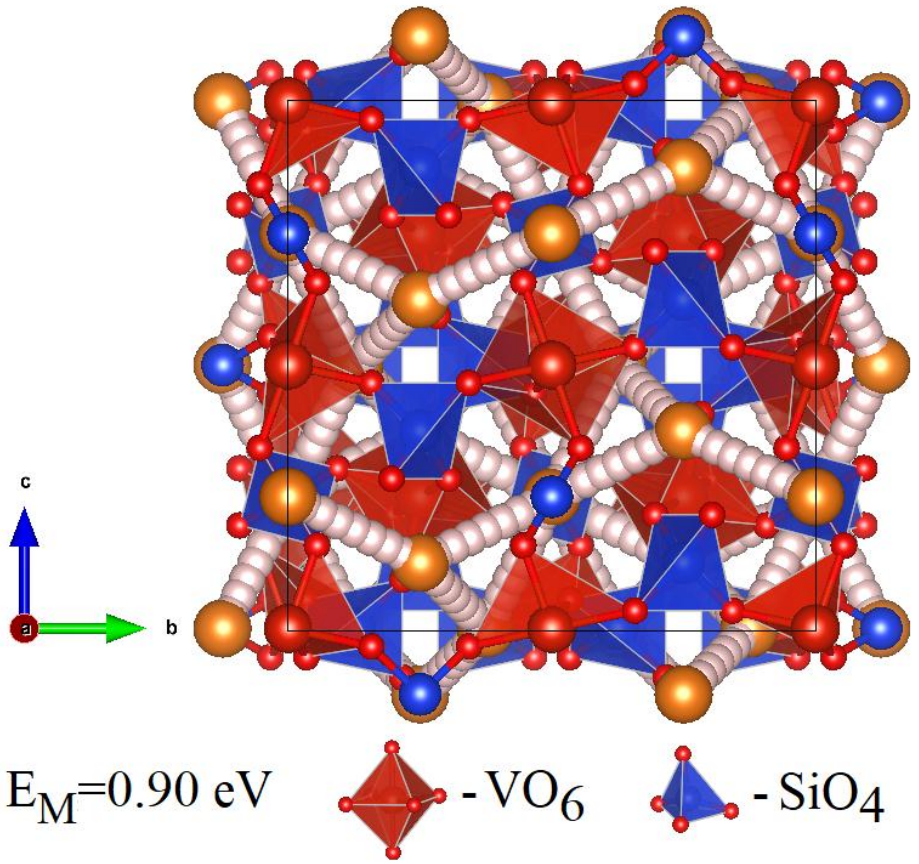
- Фотоупругие свойства

Modeling of ion conduction in solids

$$D = D_0 \exp(-E_A / kT)$$



$Mg_3V_2(SiO_4)_3$



E_M=0.90 eV - VO_6 - SiO_4

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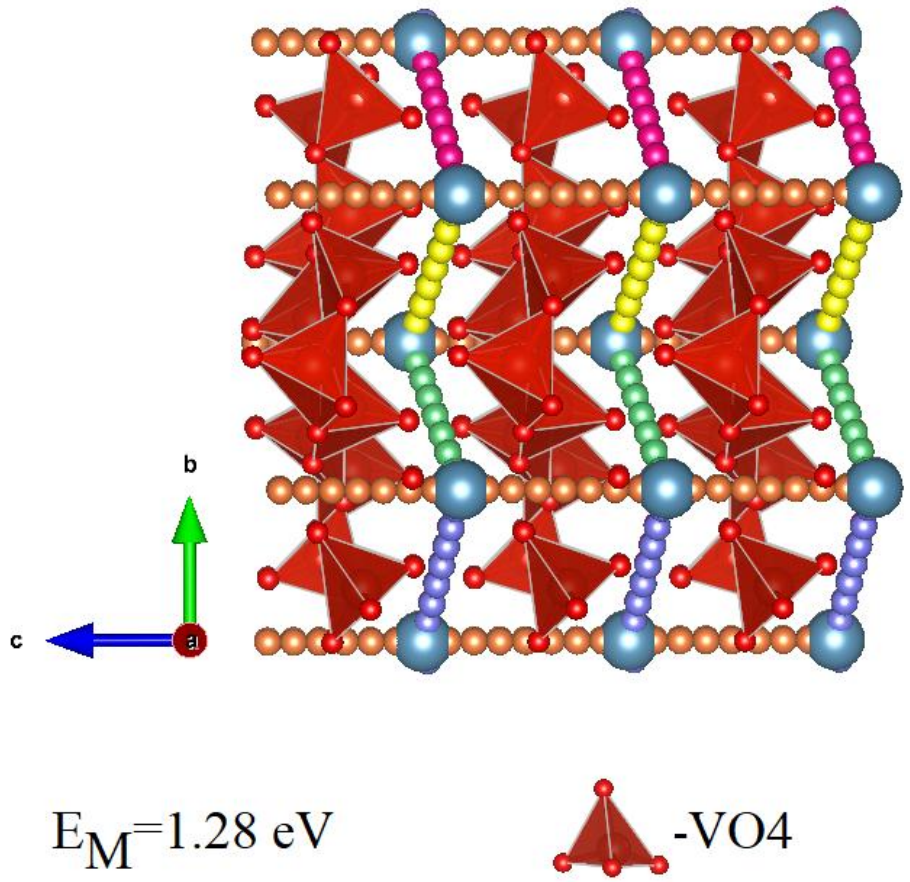
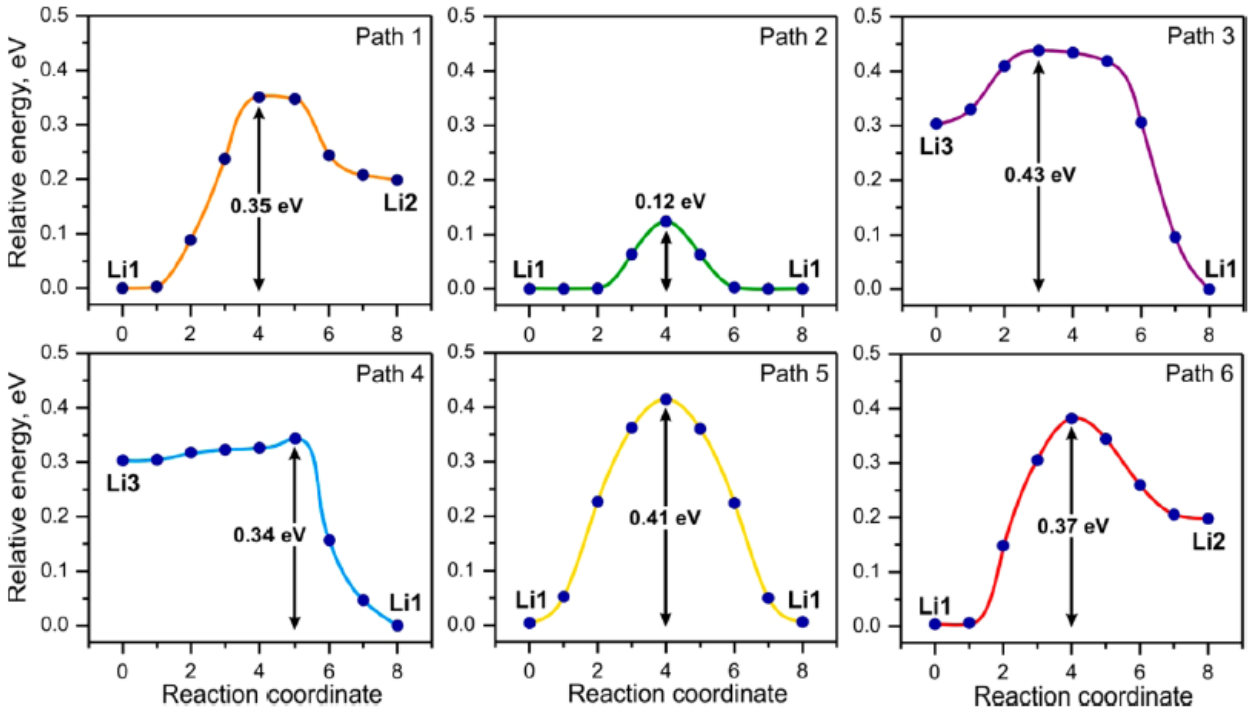
Modeling of ion conduction in solids

CaV_4O_9





E_M=1.28 eV

-VO4

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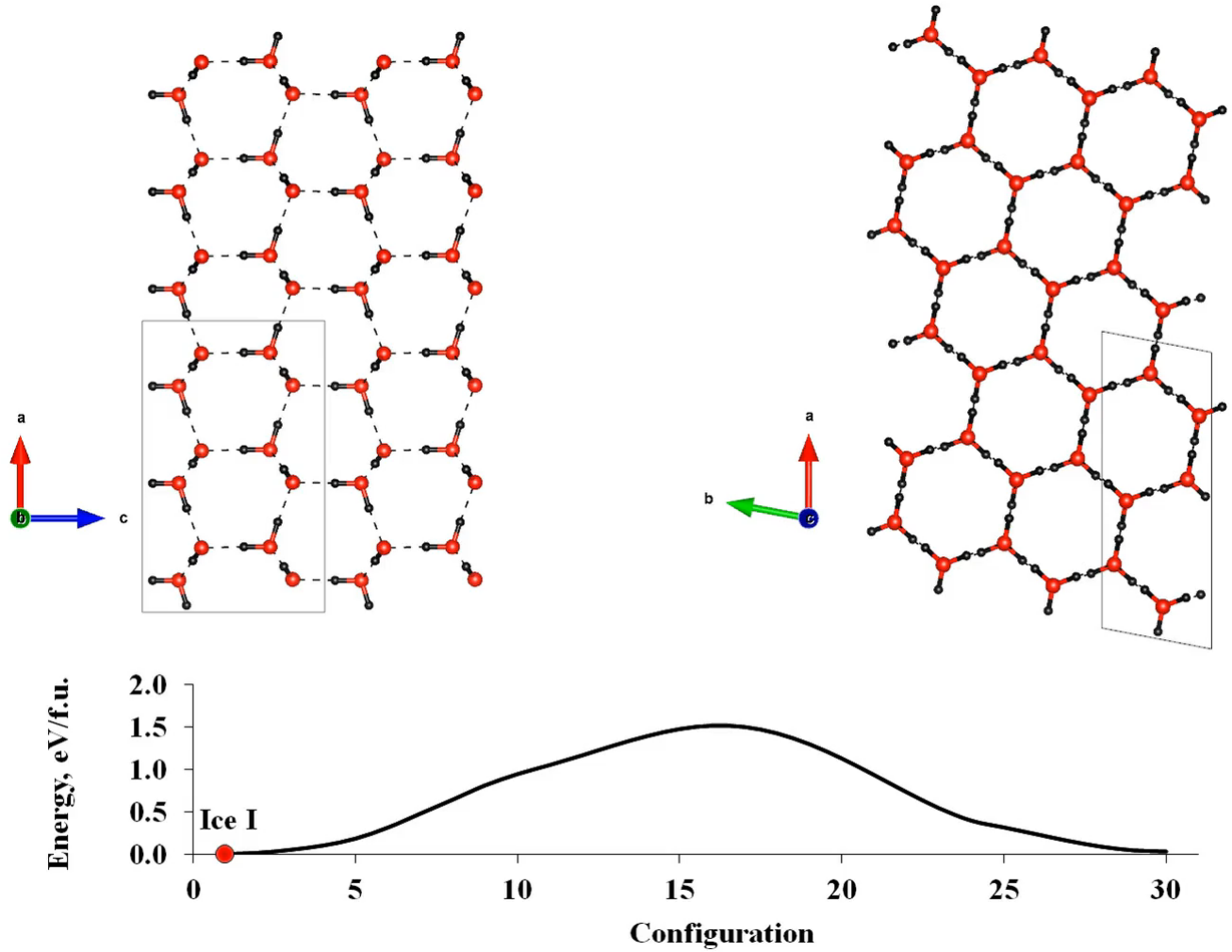
Simulation of phase transition. Ice I – Ice III



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Experimental verification

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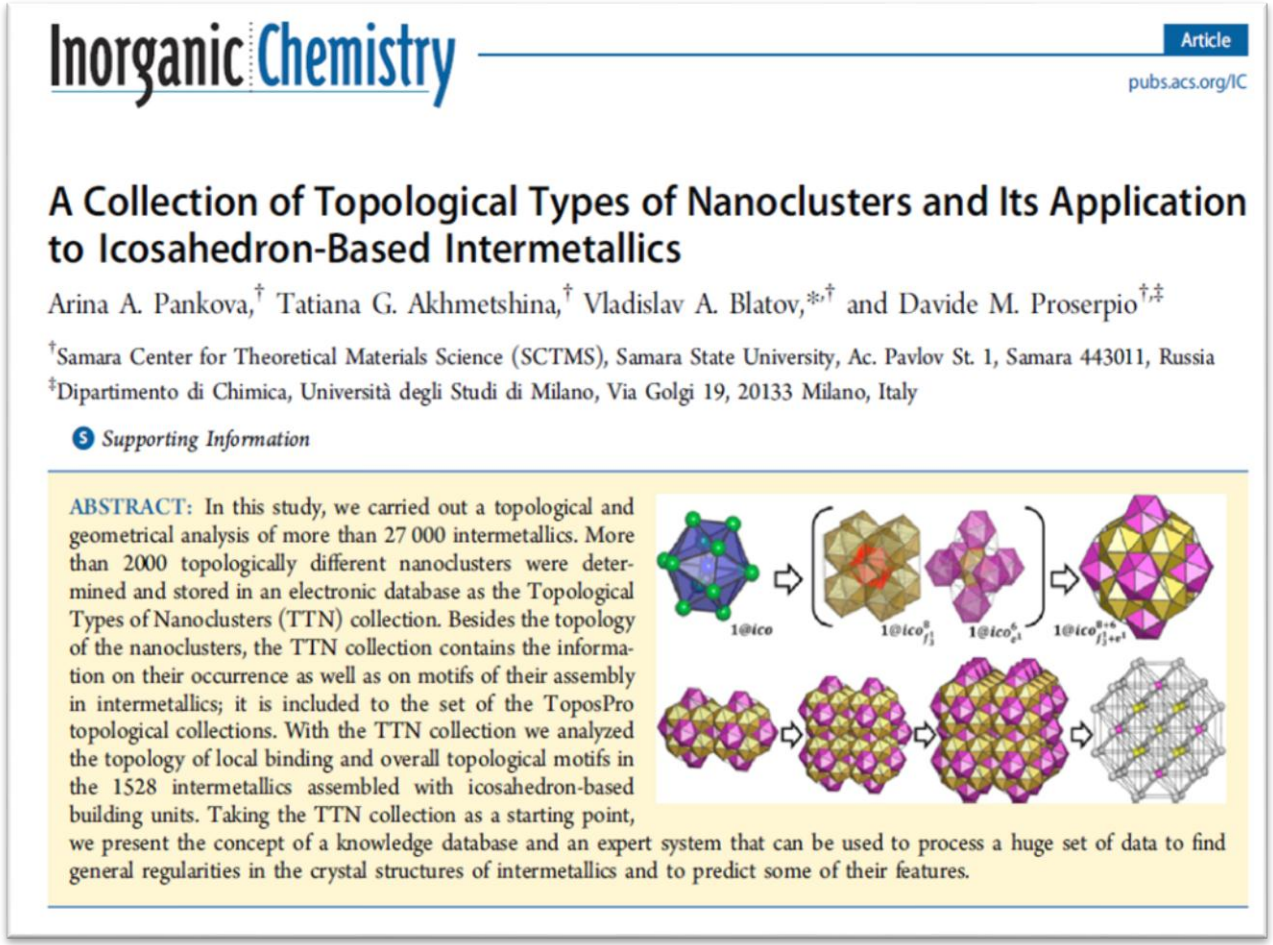
Что у нас есть?

Базы данных

Алгоритмы

Сайты

Экспериментальная часть



Inorganic Chemistry

Article

pubs.acs.org/IC

A Collection of Topological Types of Nanoclusters and Its Application to Icosahedron-Based Intermetallics

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[‡]Dipartimento di Chimica, Università degli Studi di Milano, Via Golgi 19, 20133 Milano, Italy

Supporting Information

ABSTRACT: In this study, we carried out a topological and geometrical analysis of more than 27 000 intermetallics. More than 2000 topologically different nanoclusters were determined and stored in an electronic database as the Topological Types of Nanoclusters (TTN) collection. Besides the topology of the nanoclusters, the TTN collection contains the information on their occurrence as well as on motifs of their assembly in intermetallics; it is included to the set of the ToposPro topological collections. With the TTN collection we analyzed the topology of local binding and overall topological motifs in the 1528 intermetallics assembled with icosahedron-based building units. Taking the TTN collection as a starting point, we present the concept of a knowledge database and an expert system that can be used to process a huge set of data to find general regularities in the crystal structures of intermetallics and to predict some of their features.

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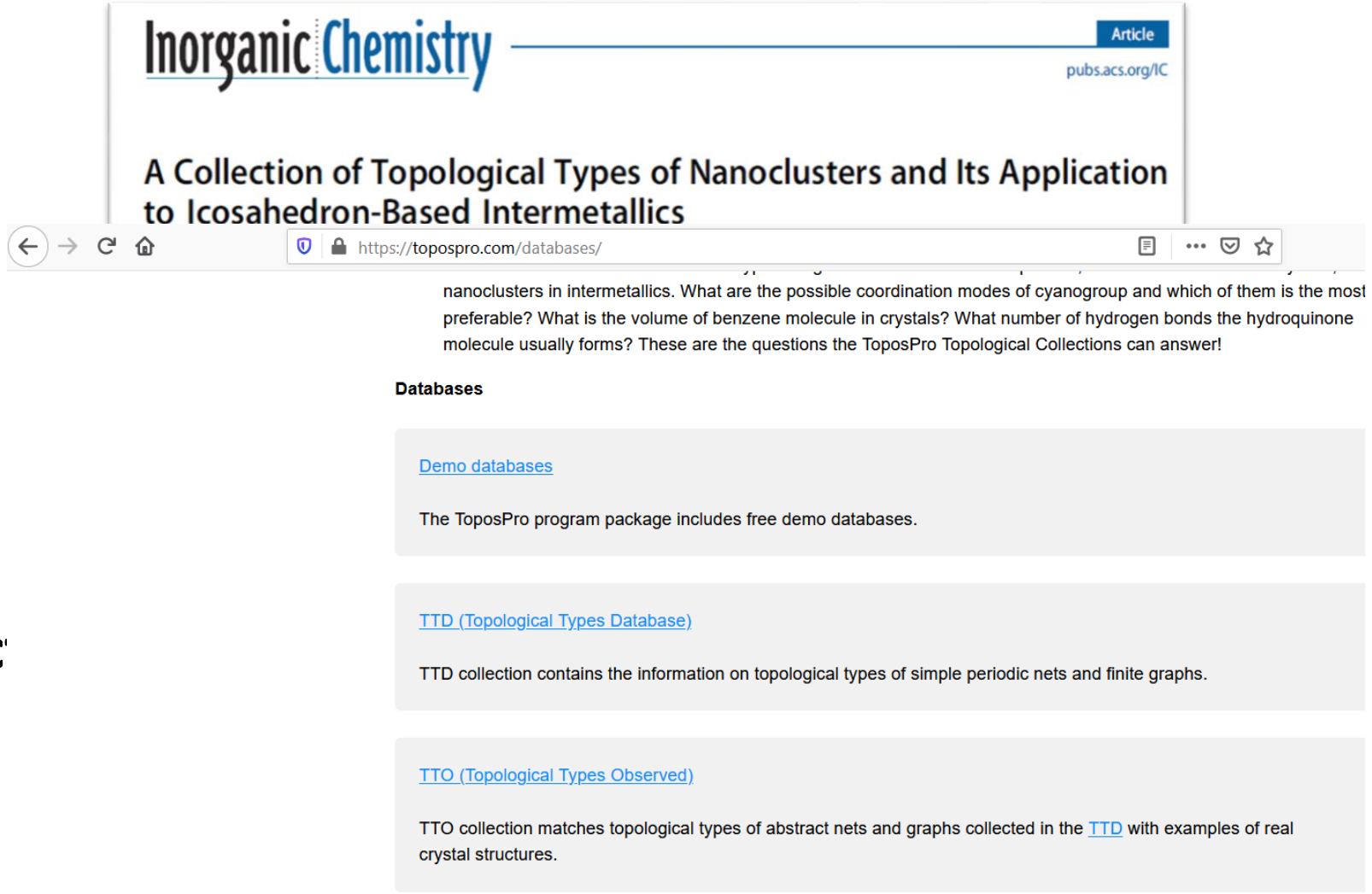

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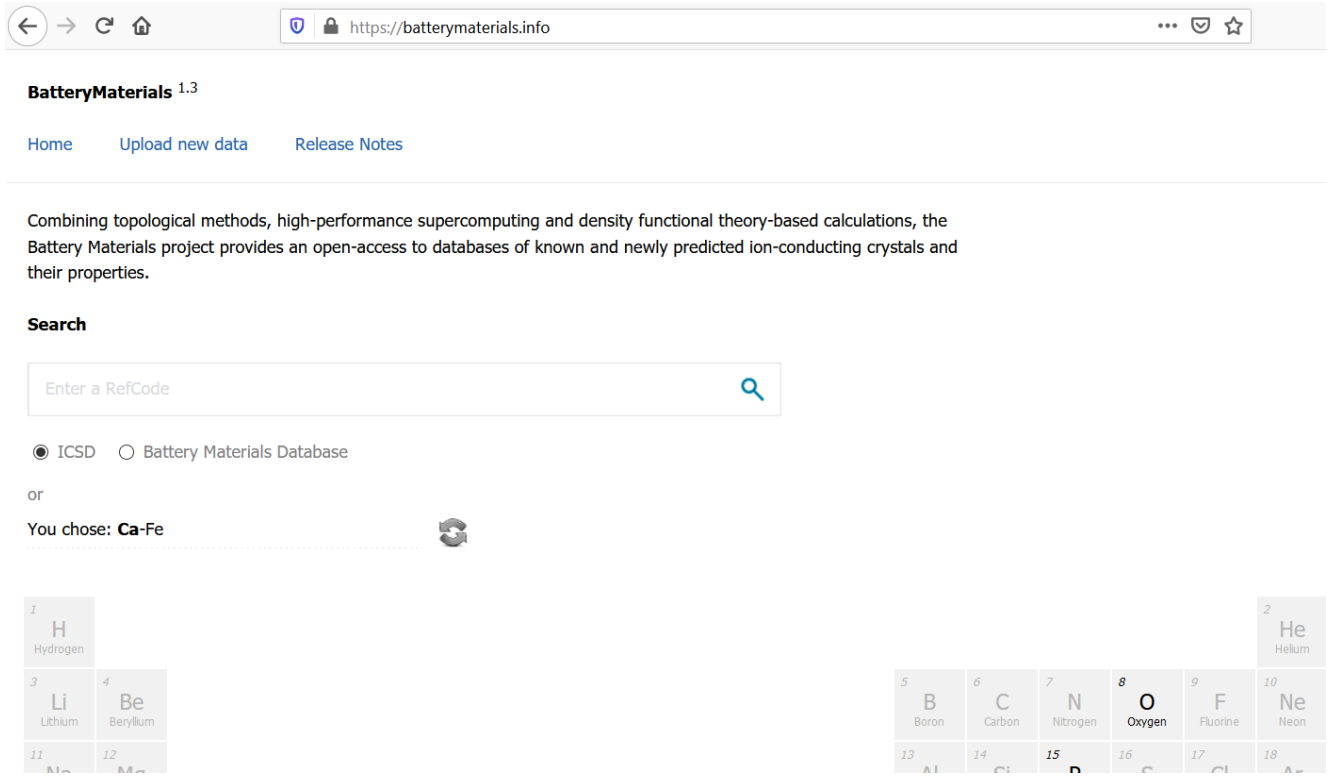

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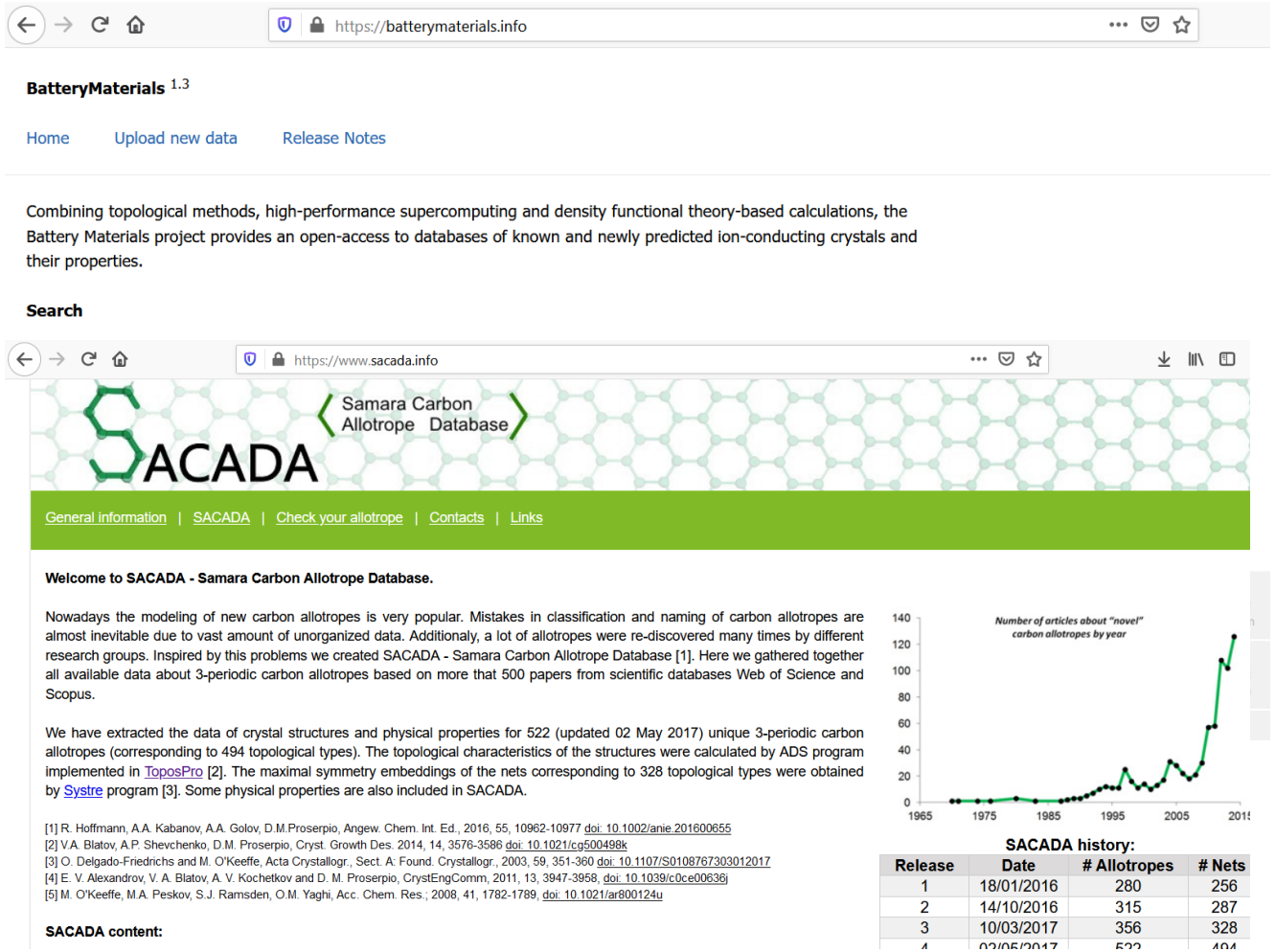

https://batterymaterials.info

BatteryMaterials 1.3

Home Upload new data Release Notes

Combining topological methods, high-performance supercomputing and density functional theory-based calculations, the Battery Materials project provides an open-access to databases of known and newly predicted ion-conducting crystals and their properties.

Search

https://www.sacada.info

SACADA Samara Carbon Allotrope Database

General information | SACADA | Check your allotrope | Contacts | Links

Welcome to SACADA - Samara Carbon Allotrope Database.

Nowadays the modeling of new carbon allotropes is very popular. Mistakes in classification and naming of carbon allotropes are almost inevitable due to vast amount of unorganized data. Additionaly, a lot of allotropes were re-discovered many times by different research groups. Inspired by this problems we created SACADA - Samara Carbon Allotrope Database [1]. Here we gathered together all available data about 3-periodic carbon allotropes based on more that 500 papers from scientific databases Web of Science and Scopus.

We have extracted the data of crystal structures and physical properties for 522 (updated 02 May 2017) unique 3-periodic carbon allotropes (corresponding to 494 topological types). The topological characteristics of the structures were calculated by ADS program implemented in ToposPro [2]. The maximal symmetry embeddings of the nets corresponding to 328 topological types were obtained by Systre program [3]. Some physical properties are also included in SACADA.

[1] R. Hoffmann, A.A. Kabanov, A.A. Golov, D.M.Proserpio, Angew. Chem. Int. Ed., 2016, 55, 10962-10977 doi: 10.1002/anie.201600655
[2] V.A. Blatov, A.P. Shevchenko, D.M. Proserpio, Cryst. Growth Des. 2014, 14, 3576-3586 doi: 10.1021/cg500498k
[3] O. Delgado-Friedrichs and M. O'Keeffe, Acta Crystallogr., Sect. A: Found. Crystallogr., 2003, 59, 351-360 doi: 10.1107/S0108767303012017
[4] E. V. Alexandrov, V. A. Blatov, A. V. Kochetkov and D. M. Proserpio, CrystEngComm, 2011, 13, 3947-3958, doi: 10.1039/c0ce00636j
[5] M. O'Keeffe, M.A. Peskov, S.J. Ramsden, O.M. Yaghi, Acc. Chem. Res.; 2008, 41, 1782-1789, doi: 10.1021/ar800124u

SACADA content:

SACADA history:

Release	Date	# Allotropes	# Nets
1	18/01/2016	280	256
2	14/10/2016	315	287
3	10/03/2017	356	328

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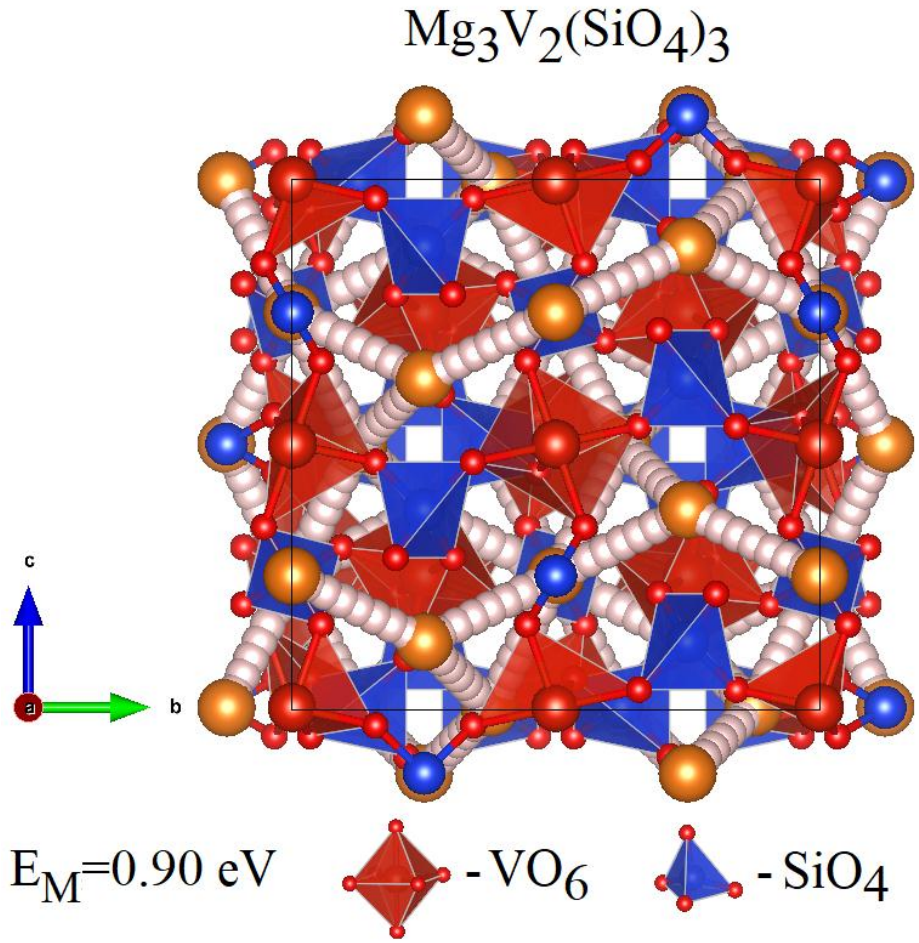

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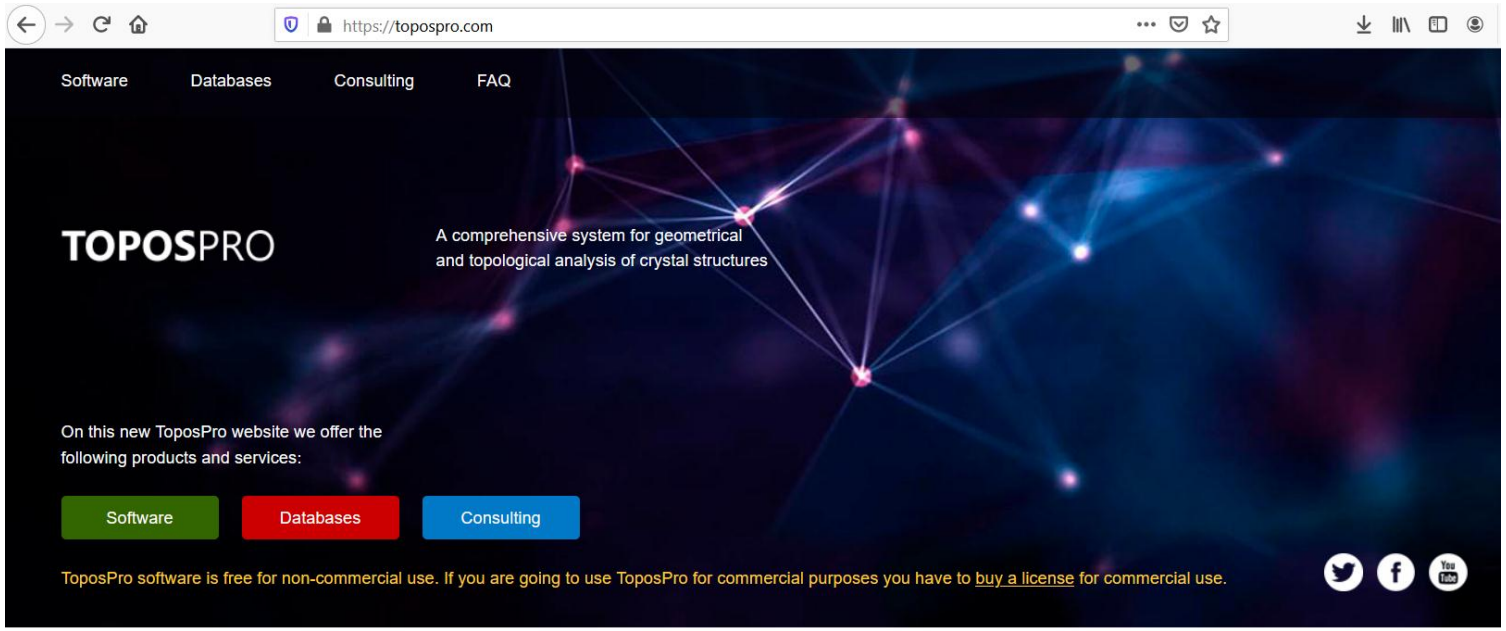

Topcryst.com - free service for determining the underlying topology of your crystal structure

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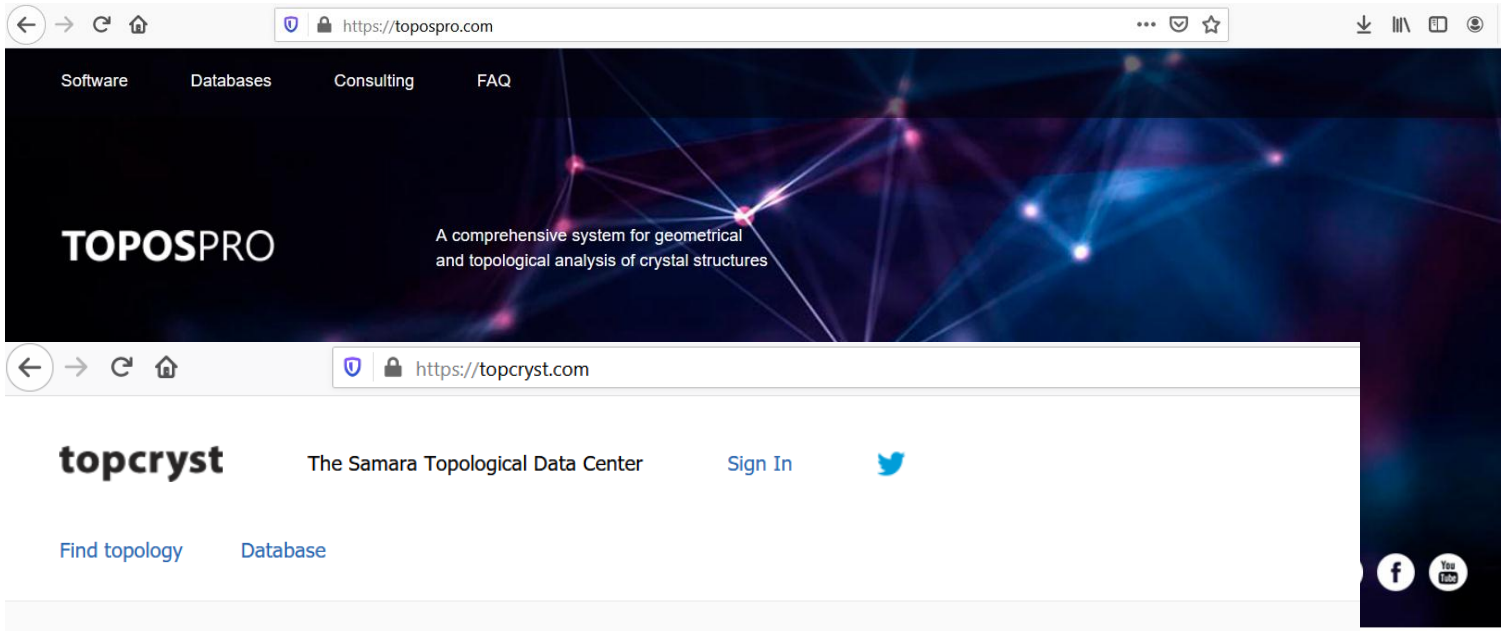

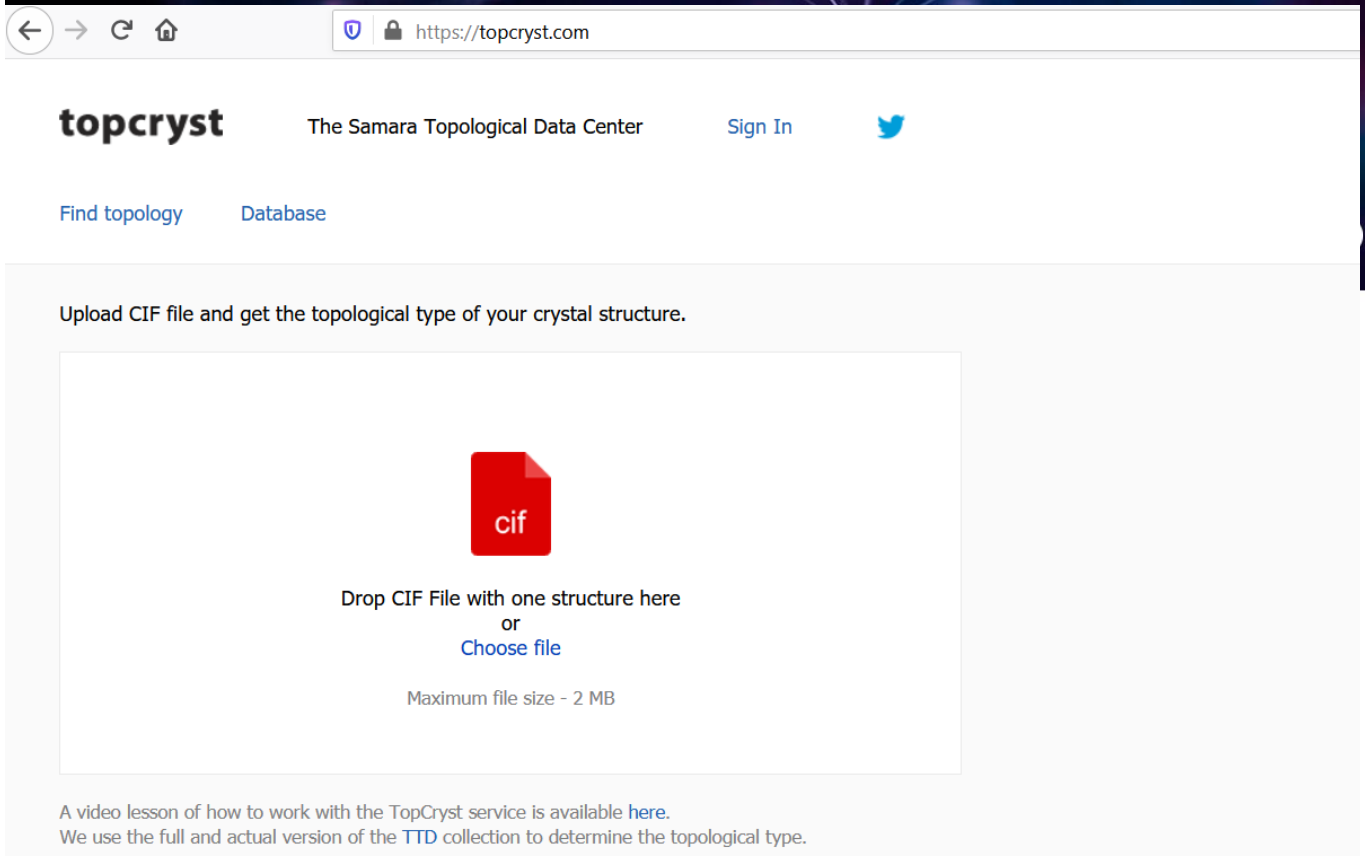

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Какая работа у нас есть?

Сбор данных (анализ статей, анализ результатов расчётов и пр.)

Обработка и подготовка данных (создание различных скриптов и пр.)

Анализ данных (нейронные сети, машинное обучение, визуализация данных и пр.)

Подготовка данных для сайтов (наполнение сайтов)

Проведение расчётов методами DFT, мол. динамики и пр.

Создание и реализация «в коде» моделей физ.-хим. процессов

Экспериментальная работа

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Спасибо за внимание

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