

Crystallography and Crystal Chemistry
X International School-Conference of
Young Scientists 2025

Mini-lecture 2: High performance computing in materials science

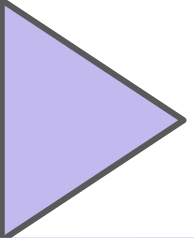
Dr. Anton Boev, PhD Arseniy Burov

PhD Maria Solovieva, PhD Daniil Chernyshov

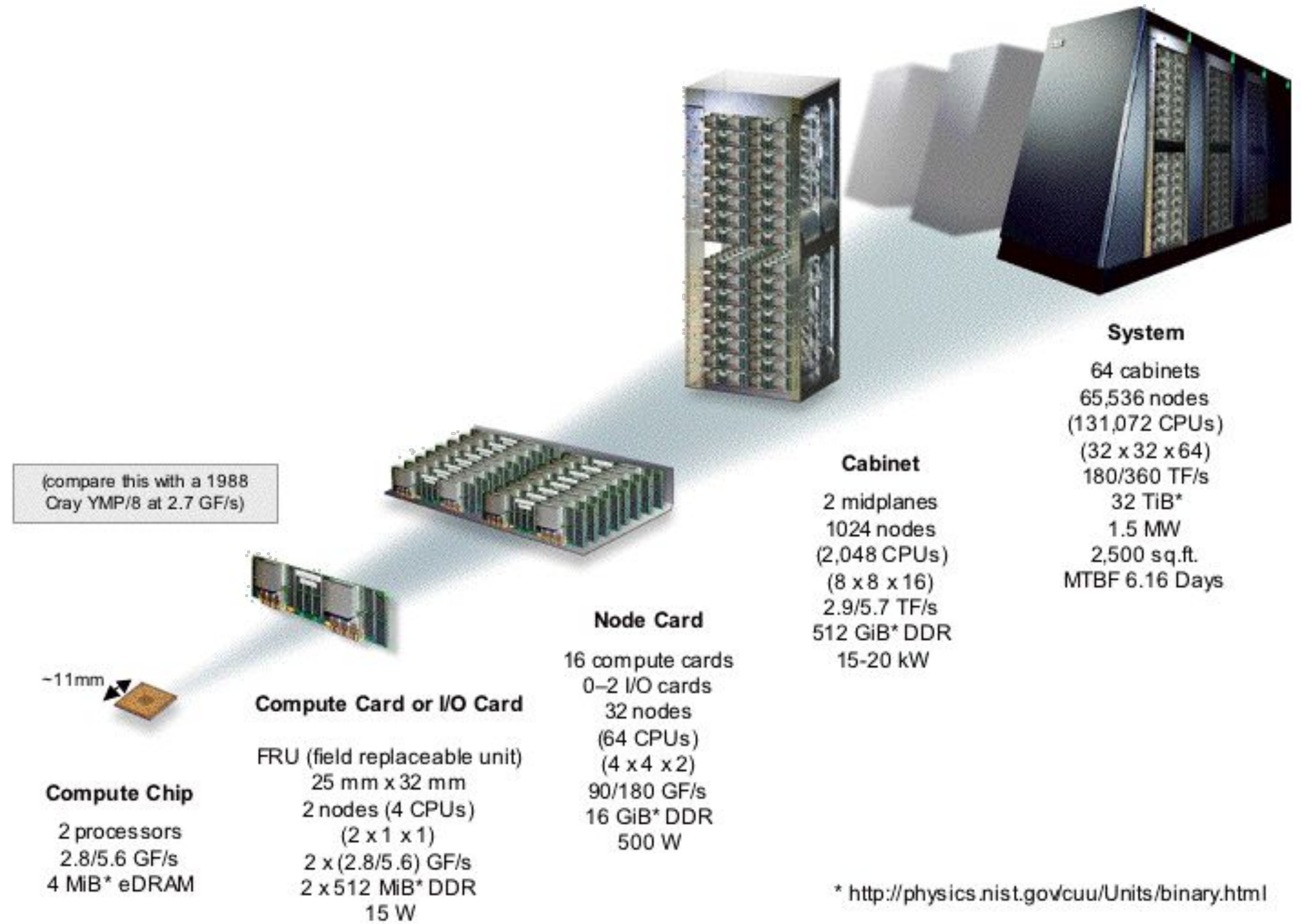
PhD Nikita Davydov, MSc Ilya Kraev

Skoltech Center for
Energy Science
and Technology

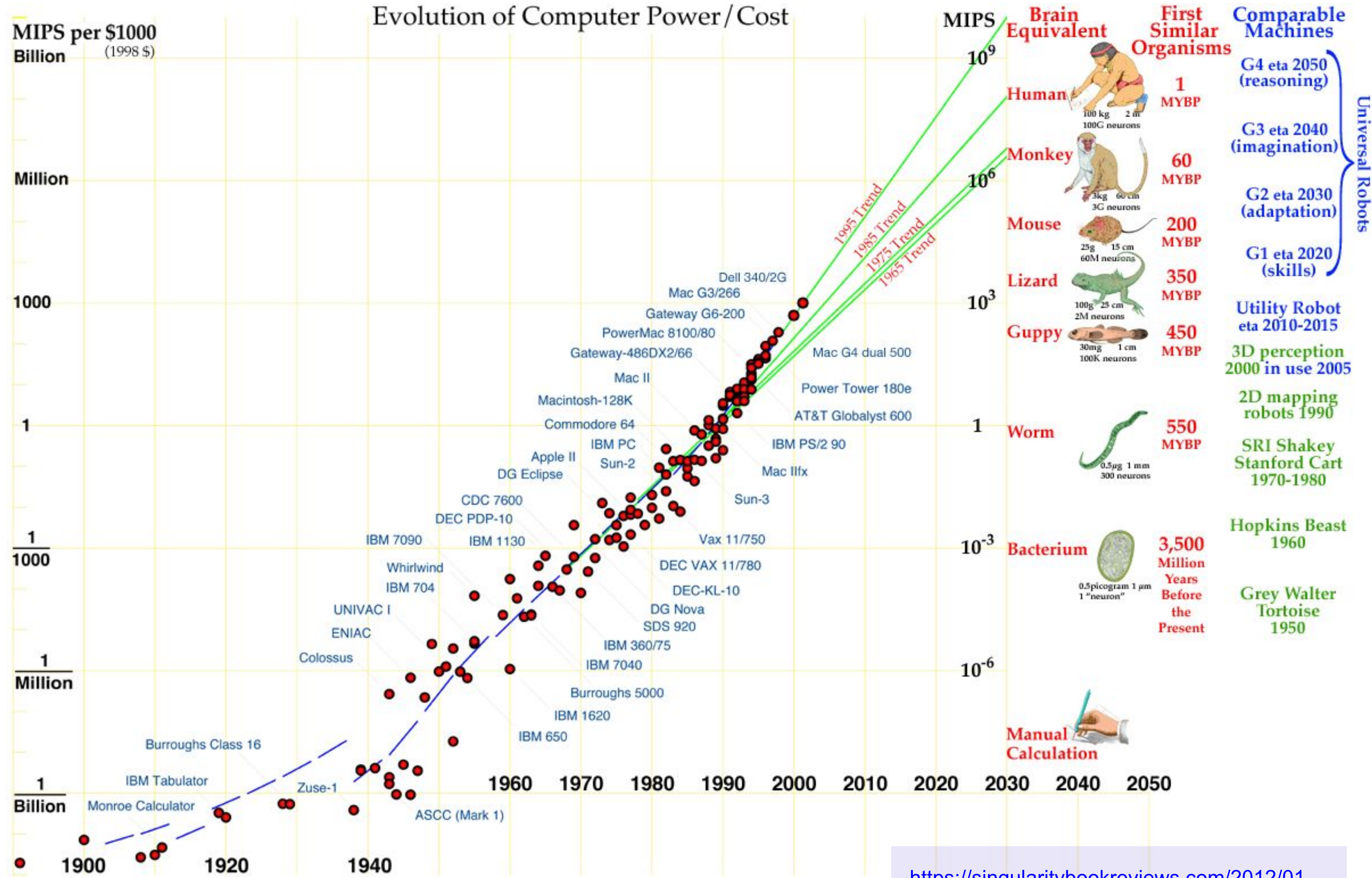
November, 2025

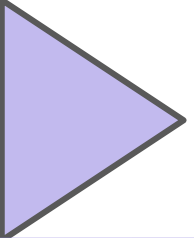


Local computer → Jupyter → Cluster



CPU power/cost evolution





Time flies...

2 M



0,4 M



2010. Вычислительный 64-х процессорный кластер Т-платформы для математических и инженерных расчетов

2020. Titan W522 - Intel Xeon Scalable Processors for Heavy Calculations Workstation PC up to 28 cores

▶ Calculation of the vacancy formation energy in aluminium (1988)

4.2. *The ideal vacancy*

We have done calculations on the vacancy system with supercells containing 8, 16 and 27 sites (7, 15 and 26 atoms). The lattice parameter a_0 is taken in each case so that

Gillan, M. J. (1989). *Journal of Physics: Condensed Matter*, 1(4), 689.

Ab initio study of oxygen point defects in GaAs, GaN, and AlN (1996)

For the defect calculations we used 32-atom supercells, which are found to give a good convergence with respect to the system size provided that a proper k -point set is used in

Mattila *et al.*, (1996). *Physical Review B*, 54(23), 16676.

Ab-initio modelling of defects in MgO (2007)

Table 2

The formation energies from the DFT calculations for the pairs of isolated defects as a function of the system size

Number of atoms	Formation energy (eV)			
	Vacancy	Interstitial	Mg Frenkel pair	O Frenkel pair
8	7.23	20.04	13.55	13.72
64	5.65	16.35	10.07	11.93
128	5.88	16.74	10.33	12.31
180	5.97	16.58	10.35	12.17

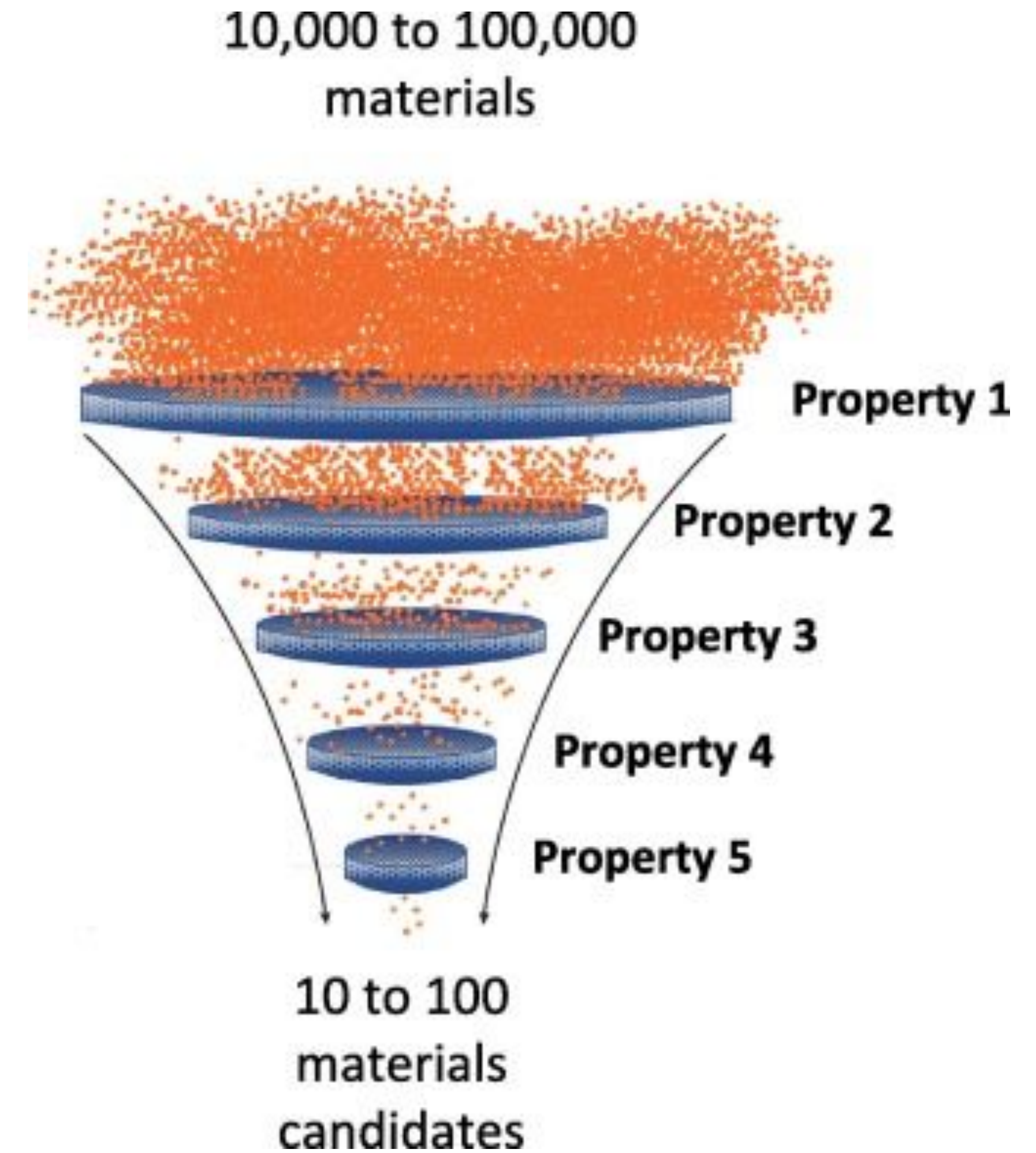
Gilbert, et al (2007). *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, 255(1), 166-171.

Interaction of Ti and Cr atoms with point defects in bcc vanadium: A DFT study (2017)

	$3 \times 3 \times 3$	$4 \times 4 \times 4$	$5 \times 5 \times 5$
Number of atoms	54	128	250
$E_f^{Vac}(at)$	2.50	2.36	2.47
	—	—	2.44 ^a
	—	—	2.51 [37]
Ω_f^{Vac}	6.2	6.9	6.6
$E_f^{\langle 100 \rangle}$	4.13	3.70	3.77
	—	3.57 [36]	—
$E_f^{\langle 110 \rangle}$	3.81	3.52	3.58
	—	3.48 [36]	—
$E_f^{\langle 111 \rangle}$	3.44	3.22	3.29
	—	3.14 [36]	—

Boev et al. (2017). *Journal of Nuclear Materials*, 492, 14-21.

High-throughput DFT screening as a nowadays trend



High-throughput screening

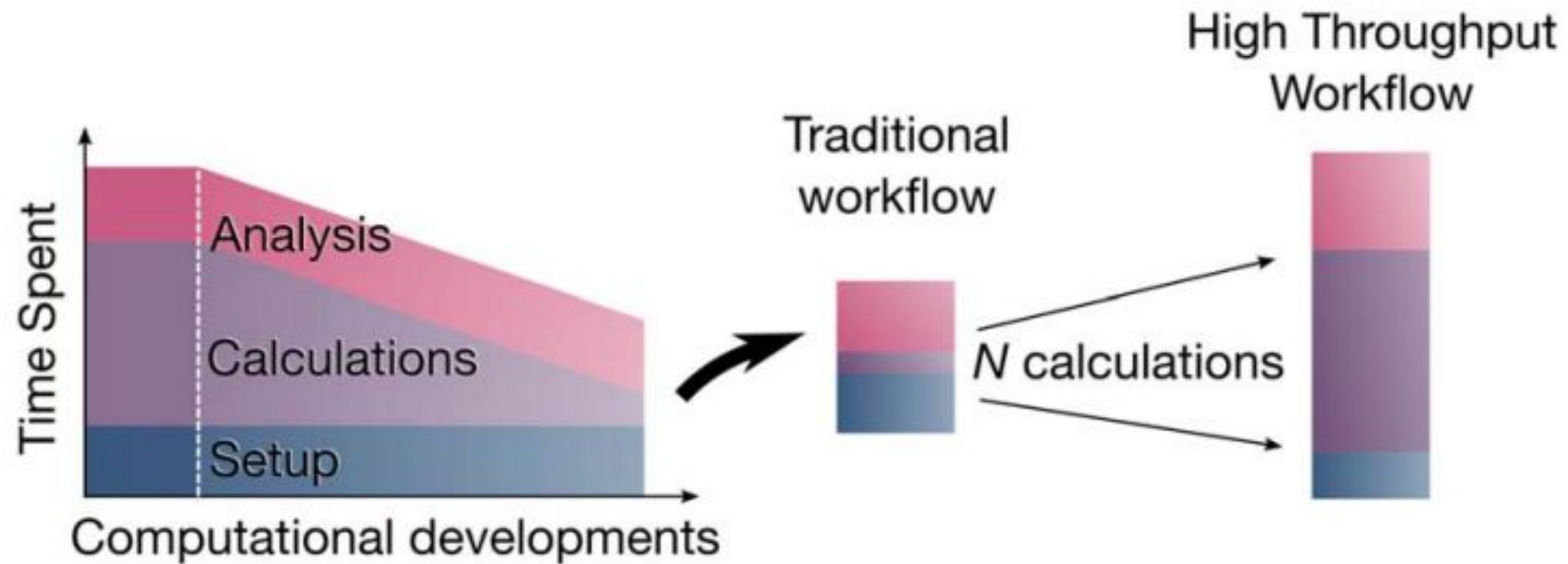


Figure 6. Time spent for calculations (and similarly for experiments) as a function of technological developments. With the computer technological advances, the calculation step can be less time consuming than the setup construction and the results analysis. Adapted from [145]. Copyright © 2018 American Chemical Society.

Schleder, *et al.* (2019). *Journal of Physics: Materials*, 2(3), 032001.

Materials project

The Materials Project by the numbers

MATERIALS

154,718

REGISTERED USERS

400,000+

INTERCALATION ELECTRODES

4,351

CITATIONS

19,000+

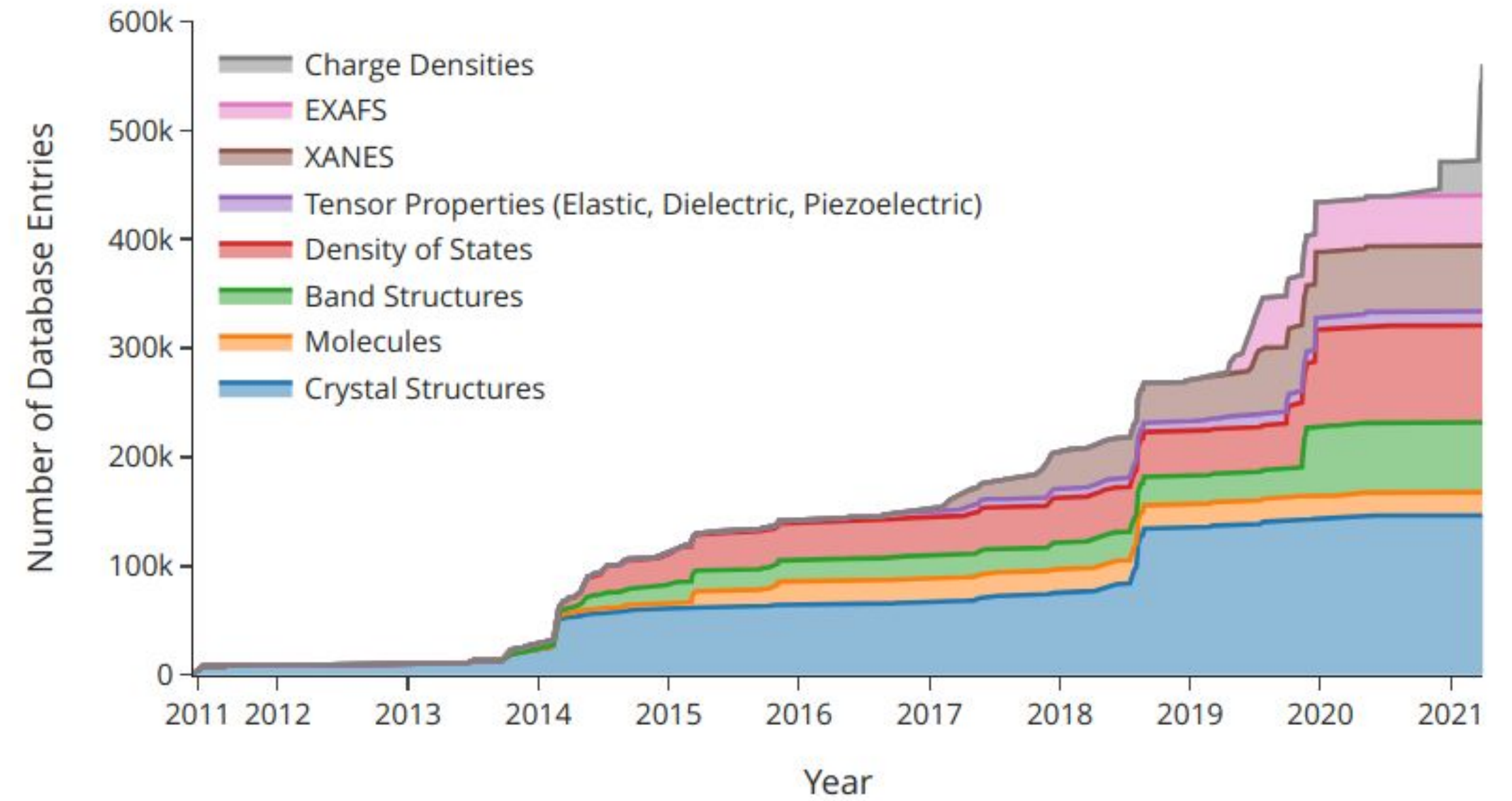
MOLECULES

172,874

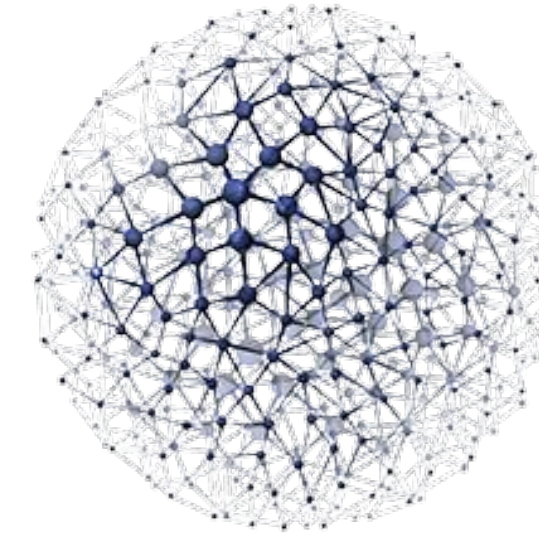
CPU HOURS/YEAR

100 million

DATABASE ENTRIES



<https://next-gen.materialsproject.org/>



Welcome to AFLOW, a globally available database of **3,530,330** material compounds with over **734,308,640** calculated properties, and growing.

3,479,057

form. enthalpies

366,988

band structures

172,488

Bader charges

5,650

elastic properties

5,664

thermal properties

1,738

binary systems

30,289

ternary systems

150,659

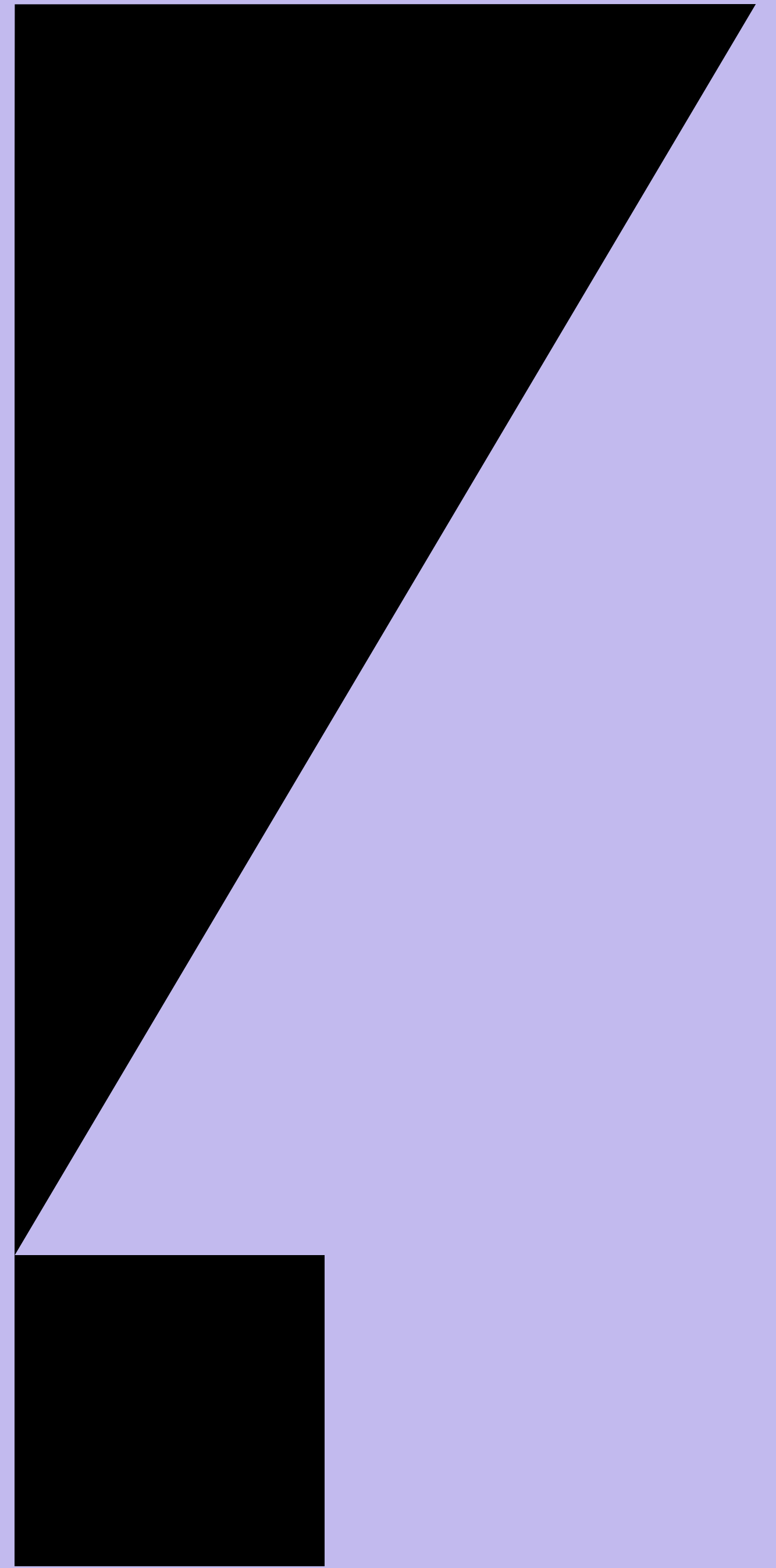
quaternary systems

<https://aflowlib.org/>

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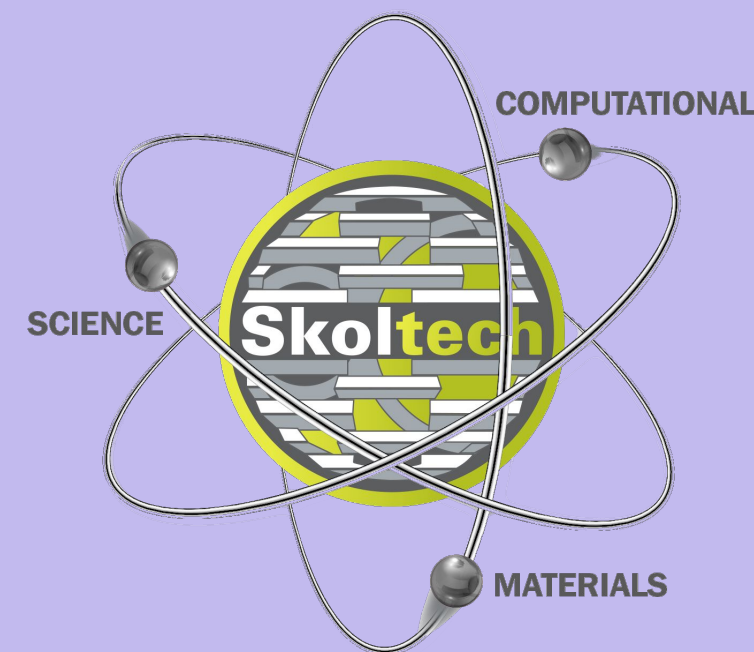
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Acknowledgement

Skoltech
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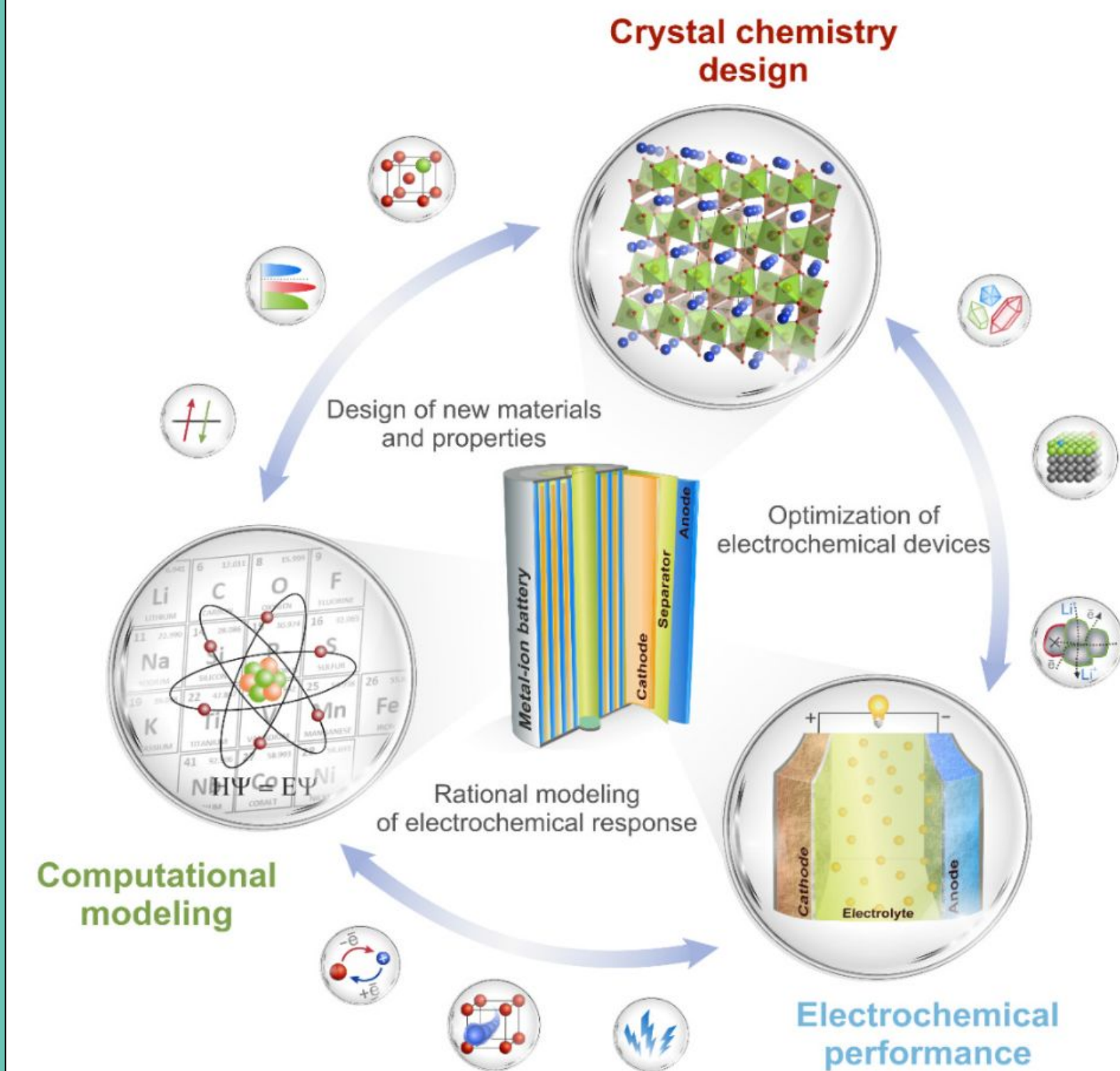


Russian Science
Foundation

Our group

Storion Research Lab

Center for Energy Science and Technology at Skoltech, Moscow



★ [MatSolver](#) - a web-service for predicting materials properties.