MISIS
National University
of Science and Technology

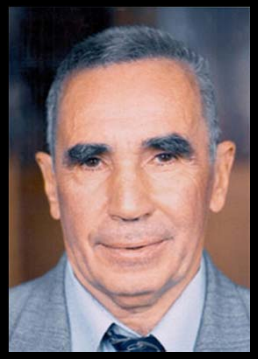
Использование современных суперкомпьютеров для теоретического моделирования и ускоренной разработки новых материалов

Лаборатория моделирования и разработки новых материалов, НИТУ "МИСиС"

Moscow, 2017

Materials Modeling and Development Laboratory
NUST ”MISIS”

Prof.
I. A. Abrikosov



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Dr. D. Shulyatiev.

Prof.
A. S. Mukasyan

A. Lugovskoy

Dr. L. Pourovsky

A. Tal

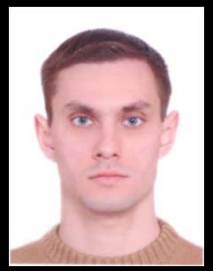
Dr. E. Smirnova

Yu. Chertov

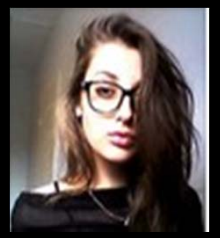
B. Muhamedov

K. Sidnov

D. Vorobyev



V. Dikan

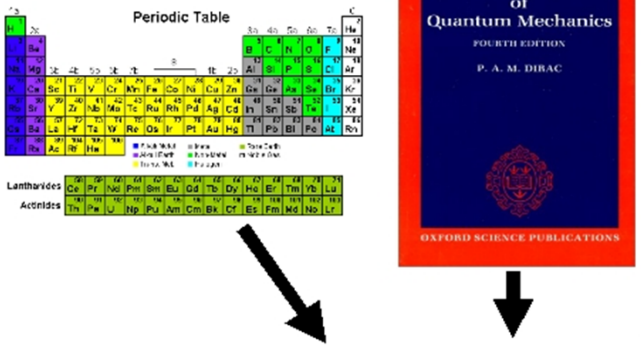


V. Kalinina

M. Klueva

Triolith@NSC,
LiU,
HP Cluster
Platform 3000
~400 TFlops

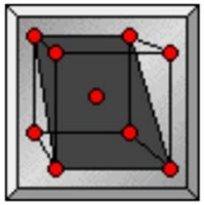
First–principles calculations



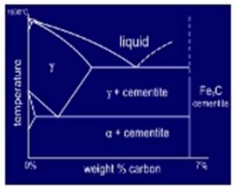
Approximations:
LDA, CPA ...
Methods:
LMTO, MD,
Monte Carlo ...

Experimental data

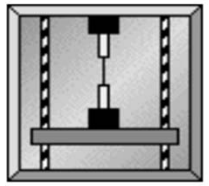
Adjustable parameters



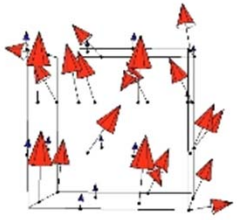
Structure



Phase equlilbria



Mechanical
properties



Magnetism

Fundamental
understanding

Supercomputer
NUST “MISIS”
HP Cluster
~38 TFlops

From quantum world towards novel materials

Theoretical physics

Basic research

Applied Studies

Quantum simulations

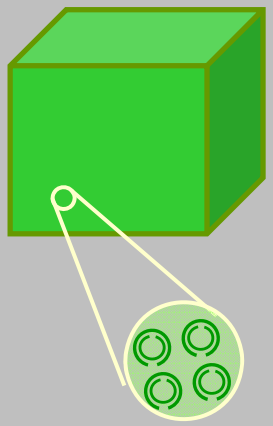
Properties vs external parameters

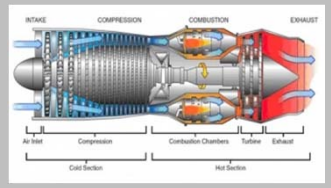
Discoveries of novel phenomena

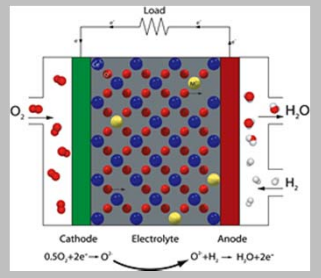
Russian key industries

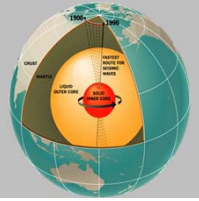
Environmentally friendly materials

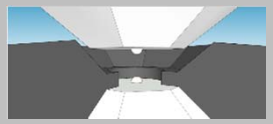
Magnetism for nano-technology

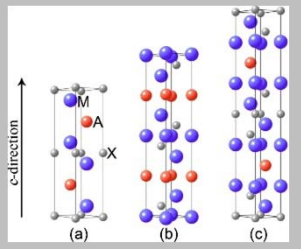




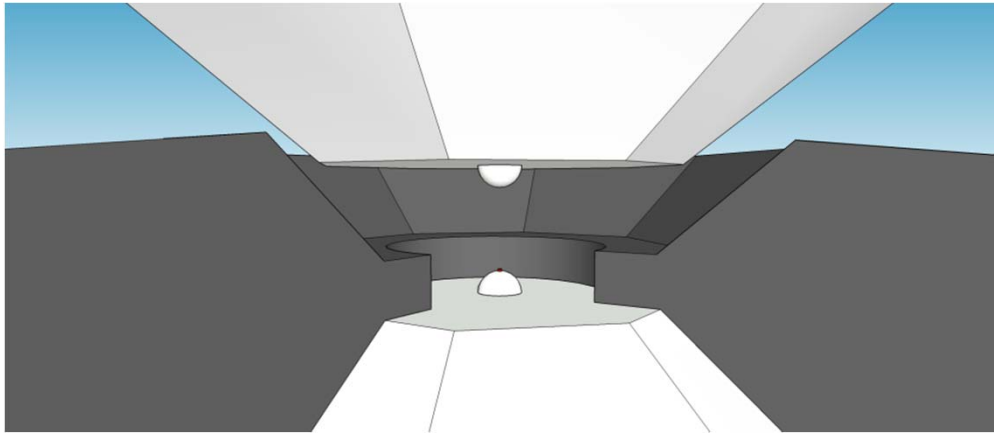


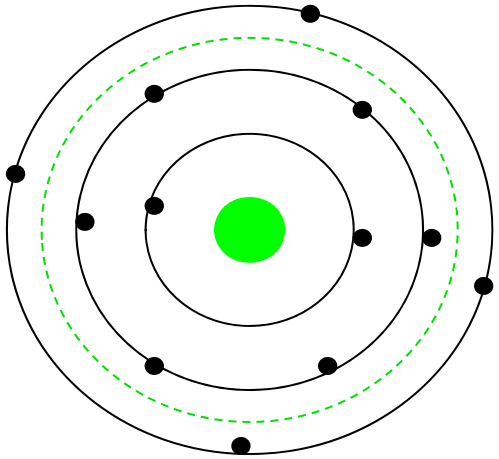




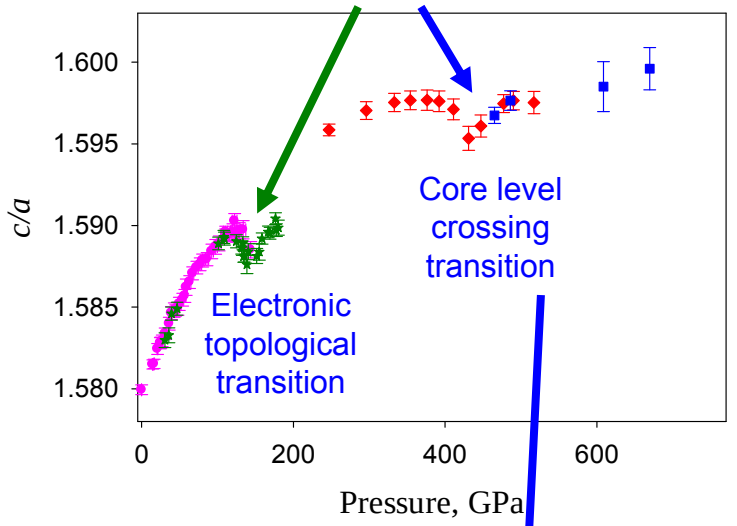


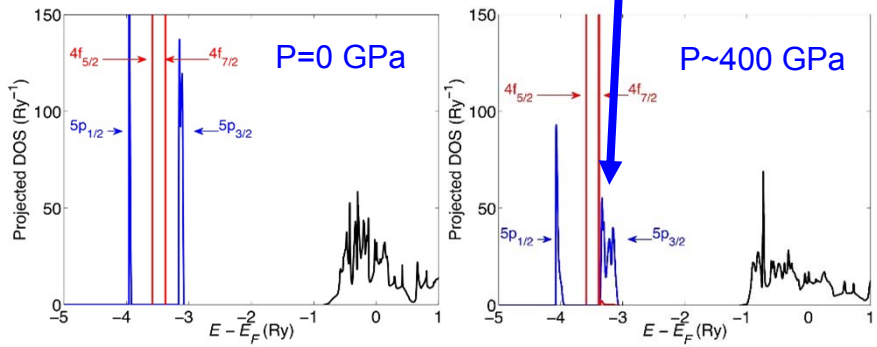
Background: fundamental studies of matter at pressure above 750 GPa, or twice as high as in the Earth's core





Experiment shows peculiarities of pressure dependence of c/a lattice parameters ratio in hcp Os.



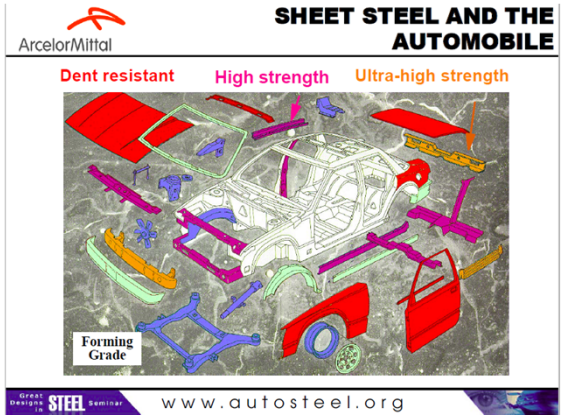


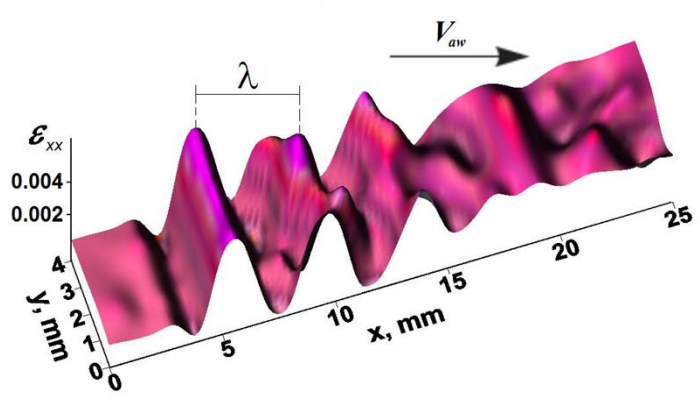
Theory explains them discovering electronic transitions in Os upon compression

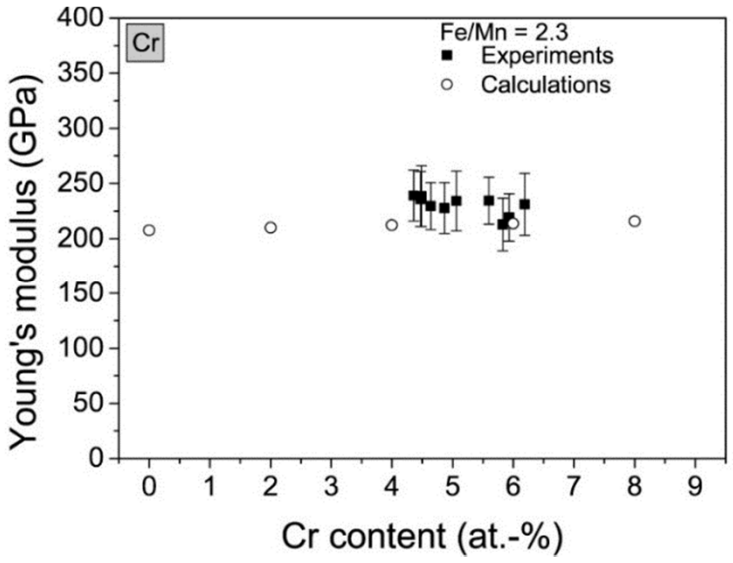
L. S. Dubrovinsky, …, I. A. Abrikosov, Nature 525, 226–229 (2015)

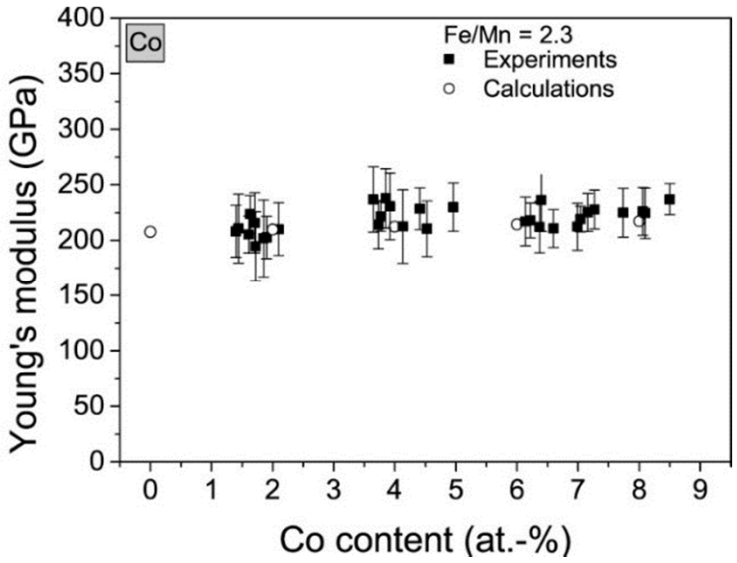
Background: theory confirms experiment

Mechanical properties of high-strength steels







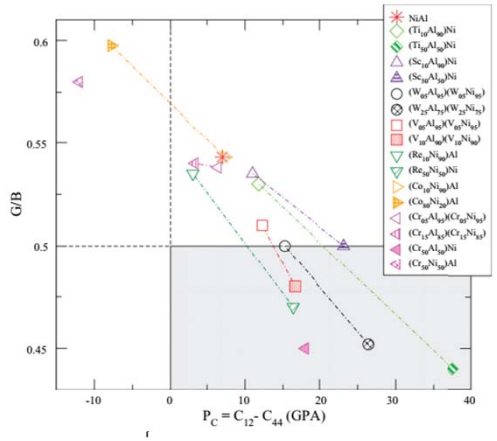


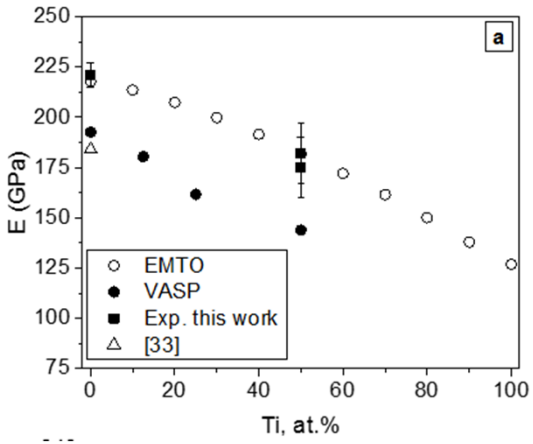
I. A. Abrikosov, A. V. Ponomareva, *et al.*, COSSMS **20**, 85 (2016)

Background: theory motivates experiment

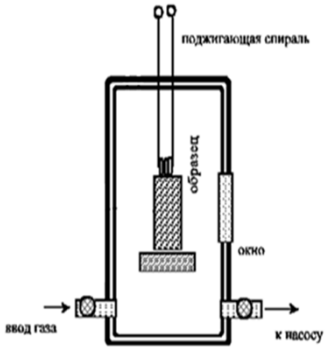
Novel NiAl-X alloys

Theory

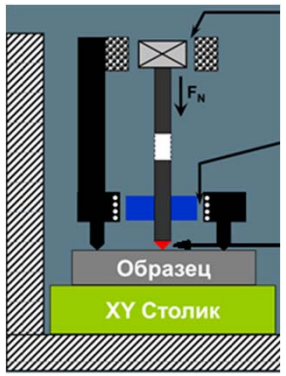


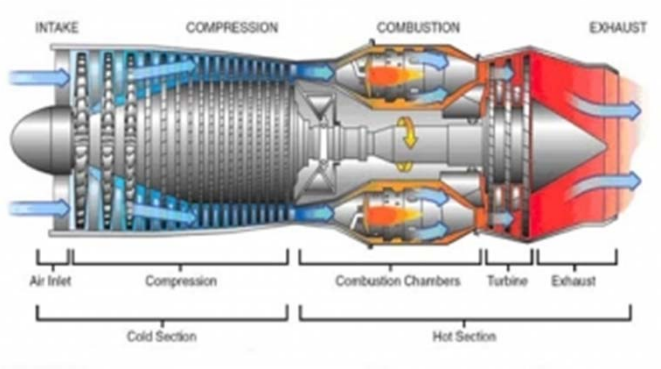


Synthesis



Characterisation

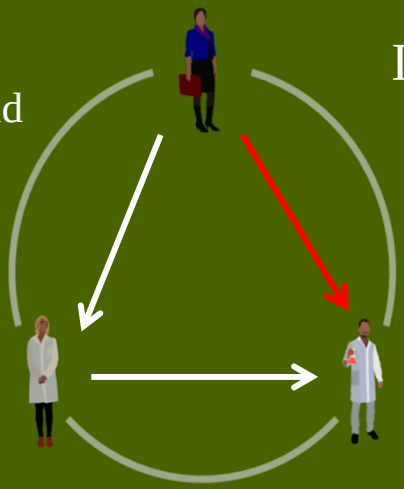




K. Sidnov,…, A. V. Ponomareva, I. A. Abrikosov, …, A. S. Mukasyan, J. Alloys Comp. **688**, 534 (2016)

How create a win-win scenario for all?

«Materials informatics and quantum synthesis» project: to reduce time to 5-6 years



Industry

Traditional materials design takes 10-12 year

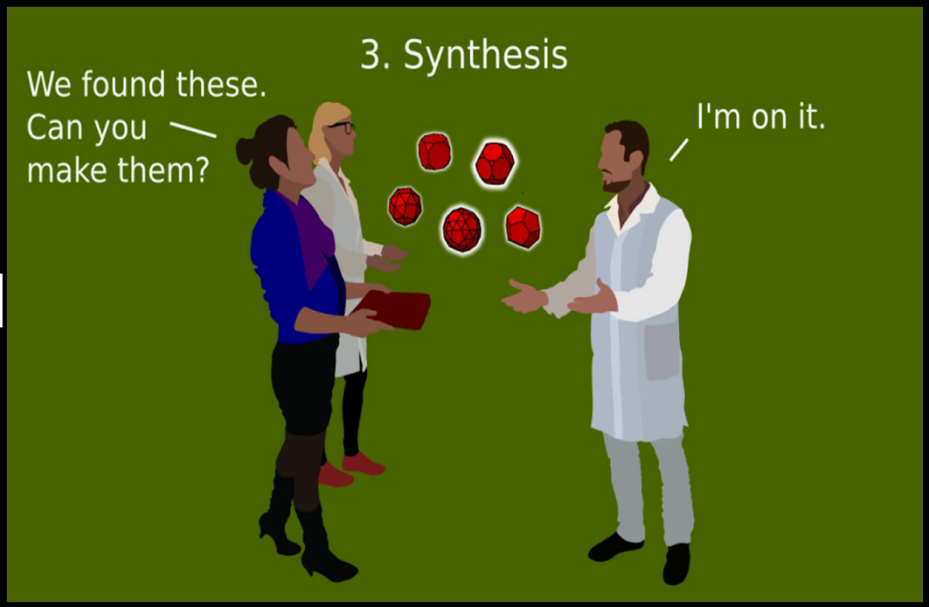
Theory

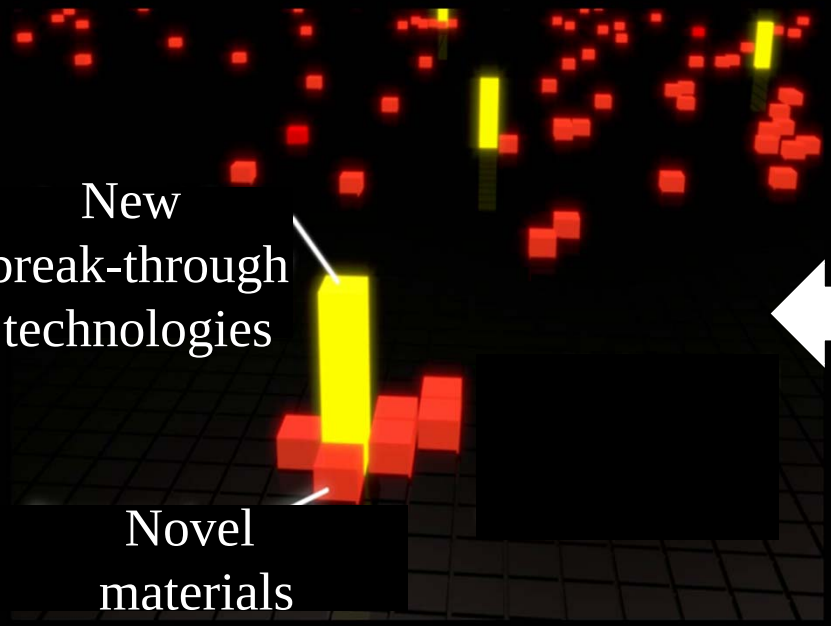
Experiment

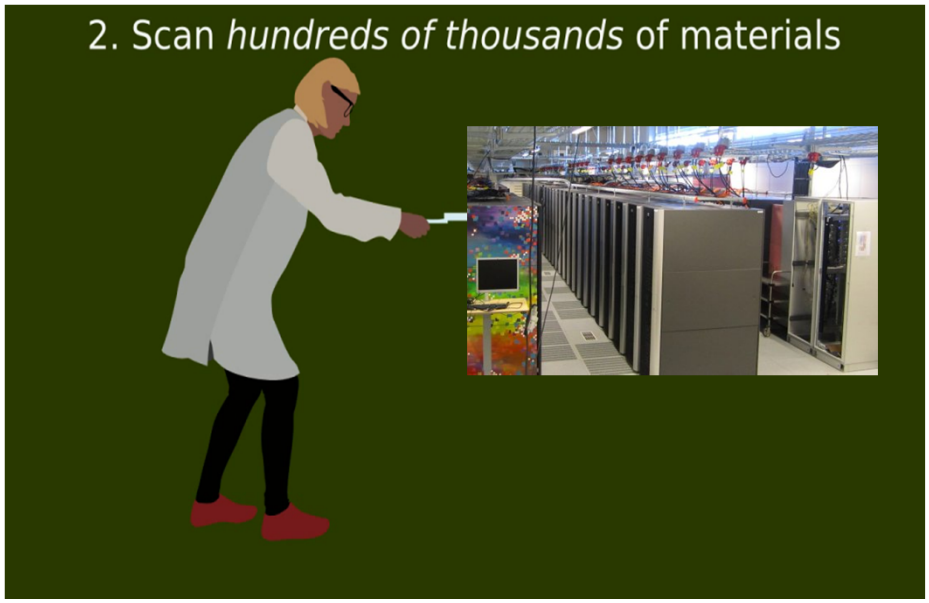
2. Scan *hundreds of thousands* of materials

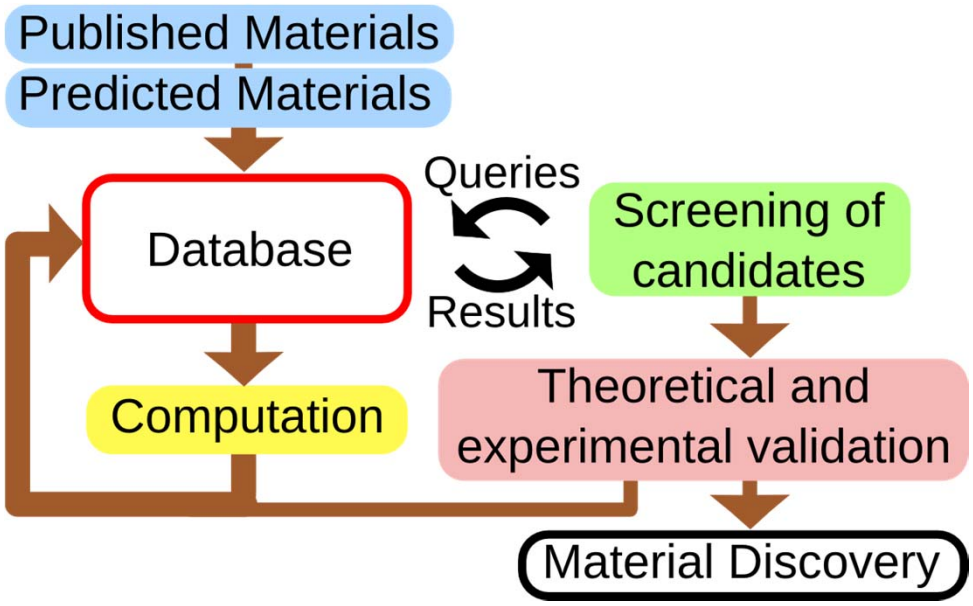
Supercomputer

3. Synthesis







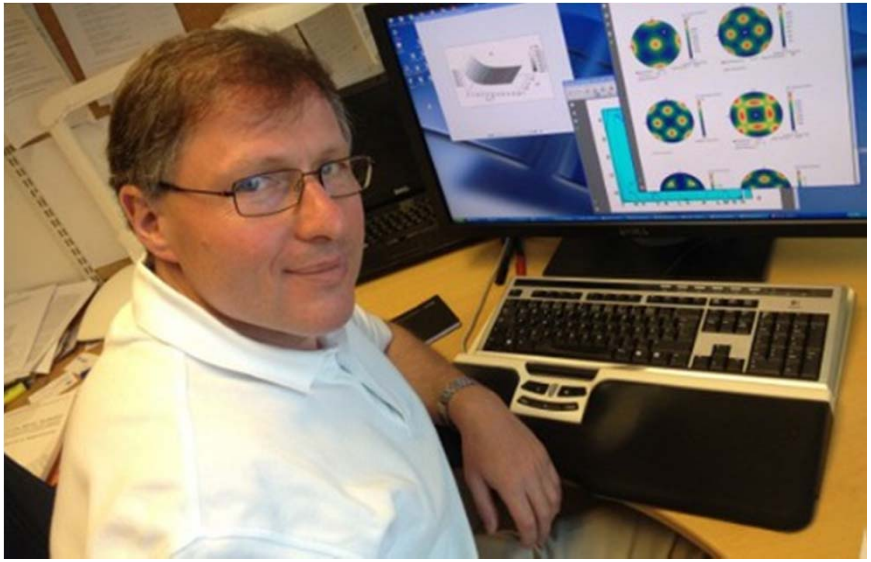


- Generate, collect, and curate Big Materials Data (BMD) from a wide range of sources.
- Explore the BMD with efficient machine learning and visualization algorithms.
- Discover novel materials, exciting phenomena, new parameter-properties and parameter-parameter relations.
- Deliver the BMD data and the generated knowledge to end users through visual decision support environments.

Cooperating with partners

Collaborating groups dealing with **quantum physics**, have a unique expertise in areas related to the quantum simulation, fabrication of qubits and quantum circuits, quantum metamaterials, theoretical methods of quantum many-body physics, electronic structure theory, materials modeling, and data-driven materials design, which is necessary to achieve the project goals.

Научный лидер проекта



Игорь Анатольевич Абрикосов

Академик Королевской Шведской Академии Наук, доктор физико-математических наук, профессор, заведующий отделом теоретической физики Института физики, химии и биологии университета Линчёпинга (Швеция), руководитель Междисциплинарной лаборатории моделирования и разработки новых материалов НИТУ МИСИС.

Область исследований профессора Абрикосова охватывает широкий спектр фундаментальных проблем в теоретической физике твердого тела, целью которых является углубленное пониманиесвойств материалов на основе фундаментальных принципов квантовой механики и использование полученного знания как в целом ряде научных дисциплин, влкючая прикладное материаловедение, так и в промышленности.