Introduction and examples of solid surfaces phenomena

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Outline

- **Introduction myself & Electronic Structure Group, scientific directions**

- **Introduction of yourself**

- **Intro to Surfaces & and some examples**

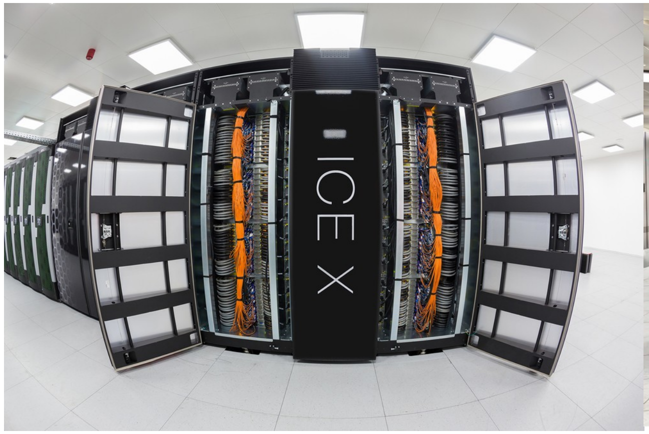
- **What does it mean surface for you?**

- **What do you investigate wrt. to surfaces/interfaces ?**

- **Which quantities, direct and indirect ones?**

- **What would be your “surface” interest? Puzzling questions? Send to dominik.legut@vsb.cz**

Czech National Supercomputing Centre - IT4Innovations



IT4Innovations – HPC center

IT4INNOVATIONS TIMELINE

Anselm

Salomon

NVIDIA DGX-2

Barbora

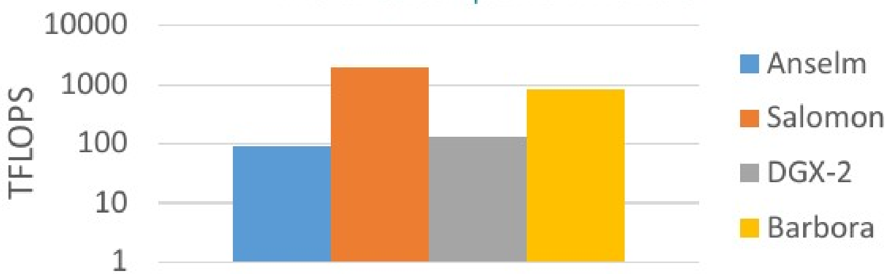
June 2013

July 2014

July 2015

March 2019

October 2019



ANSELM CLUSTER

Operational since June 2013

Theoretical performance: 94 TFLOPS

LINPACK performance: 73 TFLOPS

209 compute nodes

CPU: 2x 8-core Intel SandyBridge @ 2.3/2.4 GHz,
3322 cores total

RAM: 64 GB/96 GB/512 GB,
15 TB total

GPU: 23x NVIDIA Tesla Kepler K20

MIC: 4x Intel Xeon Phi 5110P

Storage: 320 TB/home (2 GB/s);
146 TB/scratch (6GB/s)

Network: Infiniband QDR 40 Gb/s

OS: RedHat Linux 64bit 6.x

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IT4Innovations – HPC clusters

SALOMON CLUSTER

Operational since: July 2015

Theoretical performance: 2011 TFLOPS

LINPACK performance: 1458 TFLOPS

1008 compute nodes

CPU: 2× 12-core Intel Xeon E5-2680v3 (Haswell)
@ 2.5 GHz, Turbo 3.3 GHz,
24192 cores total

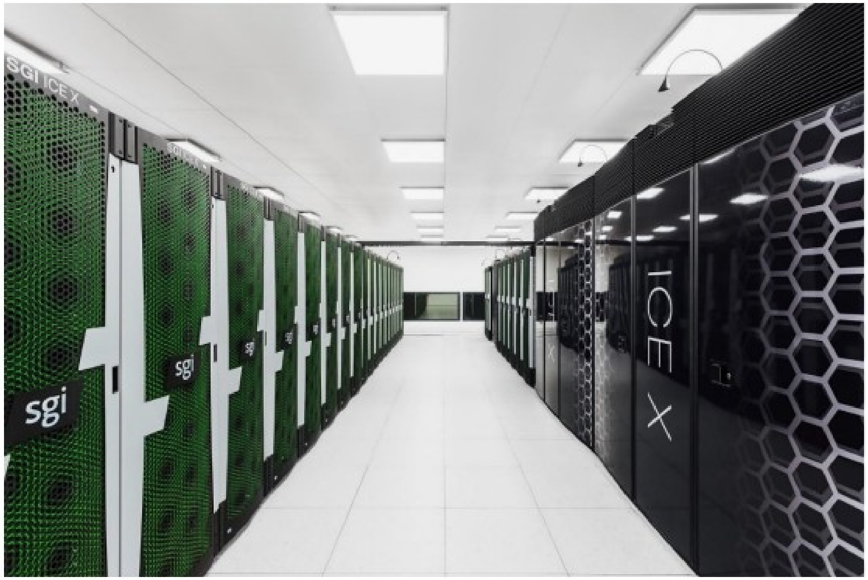
MIC: 864x Intel Xeon Phi 721P, 61 cores each,
52704 cores total

RAM: 128 GB (UV node: 3.325 TB)
129 TB total

Storage: 500 TB/home (6 GB/s),
1638 TB/scratch (30 GB/s)

Network: Infiniband FDR 56 Gb/s
7D hypercube

OS: RedHat Linux 64bit 6.x, CentOS 64bit 6.x



VSB TECHNICAL | IT4INNOVATIONS

IT4Innovations – HPC clusters

DGX-2

Operational since March 2019

Theoretical GPU performance:
FT16: 2 PFLOPS FP32: 260 TFLOPS
FP16: 520 TFLOPS FP64: 130 TFLOPS

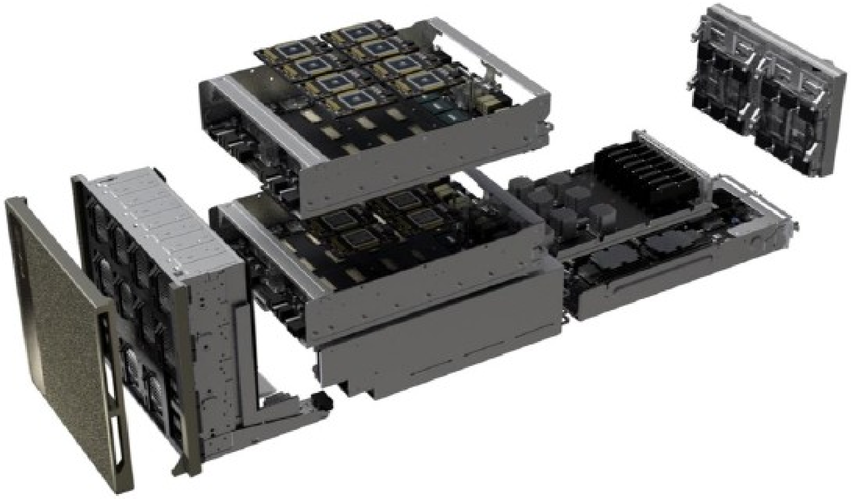
CPU: 2× 24-core Intel Xeon Platinum 8168 (Skylake)
@ 2.7 GHz, Turbo 3.7 GHz,

GPU: 16× NVIDIA V100-SXM3 (350 W),
5120 CUDA cores + 640 tensor cores
32 GB HBM2 (900 GB/s), 512 GB total
NVLink interconnect (300 GB/s)

RAM: 1.5 TB

Storage: 30 TB NVMe SSDs

Network: 8× Infiniband EDR or 100 Gb/s Ethernet



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IT4Innovations – HPC clusters

BARBORA CLUSTER

Operational since October 2019

Theoretical performance: 848 TFLOPS

192 general compute nodes
CPU: 2× 18-core Intel Xeon Gold 6240 (Cascade lake)
@ 2.6 GHz, Turbo 3.9 GHz, AVX-512 support
6912 cores in total

8 GPU accelerated nodes
CPU: 2× 12-core Intel Xeon Gold 6126 (Skylake)
GPU: 4× NVIDIA V100-SXM2, 16 GB, NVLink (50 GB/s)

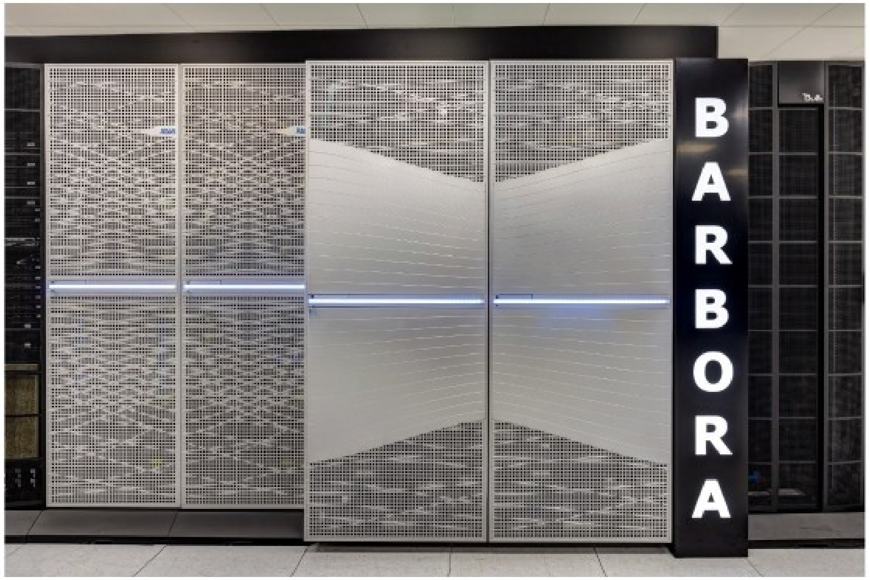
1 fat node
CPU: 8× 16-core Intel Xeon Platinum 8153 (Skylake)

RAM: 192 GB (fat node: 6 TB)
44.5 TB total

Storage: 26 TB/home (1 GB/s),
282 TB/scratch (30 GB/s),
14× 1.6 TB NVMe cache

Network: Infiniband HDR, 200Gb/s, fat tree

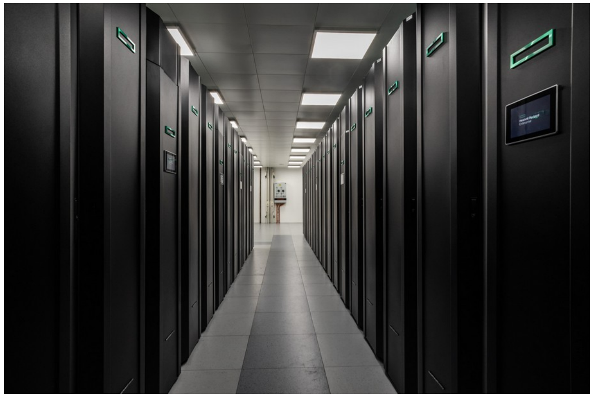
OS: RedHat Linux 64bit 6.x, CentOS 64bit 6.x



VSB TECHNICAL | IT4INNOVATIONS

IT4Innovations – HPC clusters

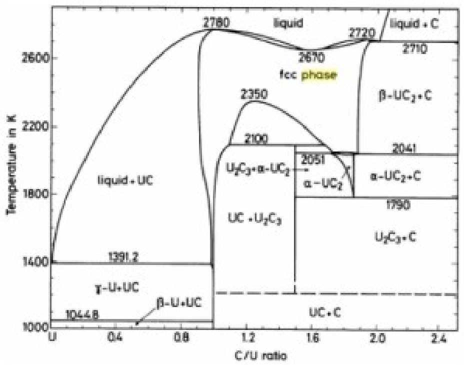
- Teoretický výkon: **15,7 PFlop/s**
- Univerzální část: **3,8 PFlop/s (LINPACK) (720 uzlů)**
- Akcelerovaná část: **11,6 PFlop/s (72 uzlů)**
  360 PFlop/s pro výpočty umělé inteligence

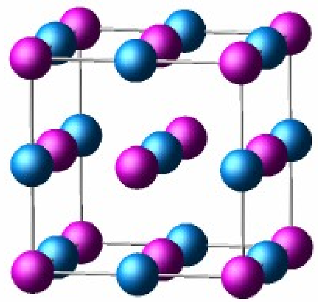


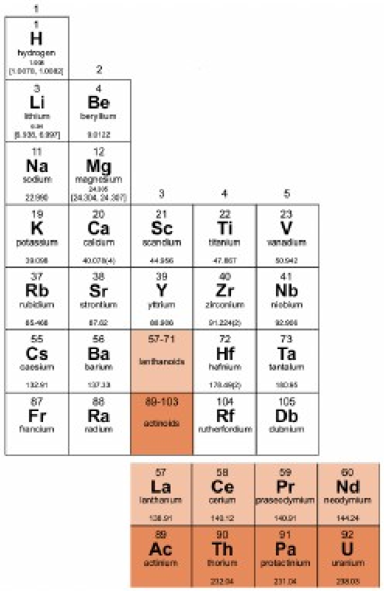
- Část pro datové analýzy: **0,071 PFlop/s, 24 TB RAM**
- Cloudová část: **192 TFlop/s (LINPACK) (36 serverů)**
- Datové uložiště: **1,4 PB** pro vysokorychlostní zpracování uživatelských dat rychlostí **až 1 TB/s**

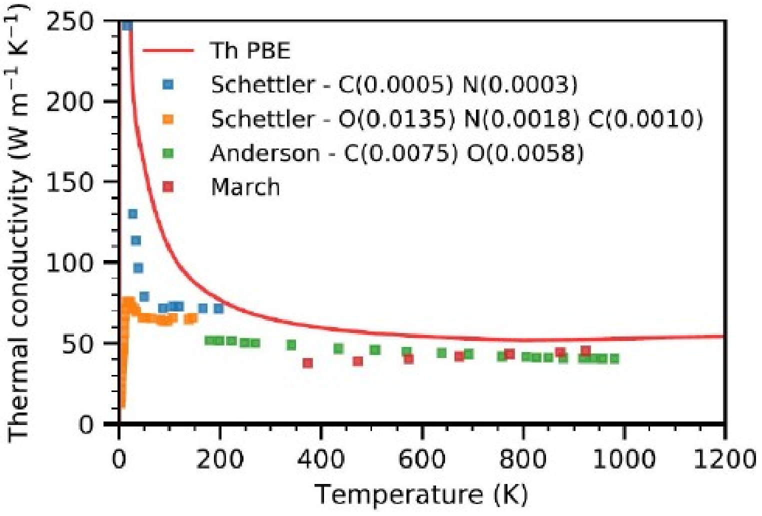
Material Design Towards Reality – www.md-esg.eu

Group leader Dr. Dominik Legut – expert in DFT and lattice dynamics simulations



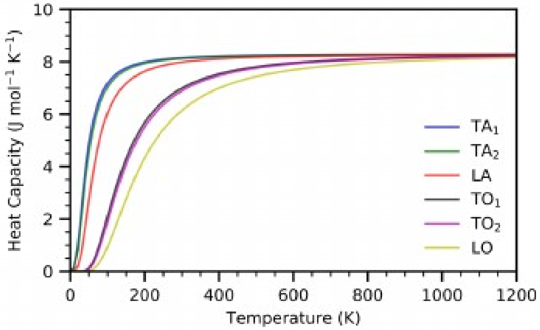


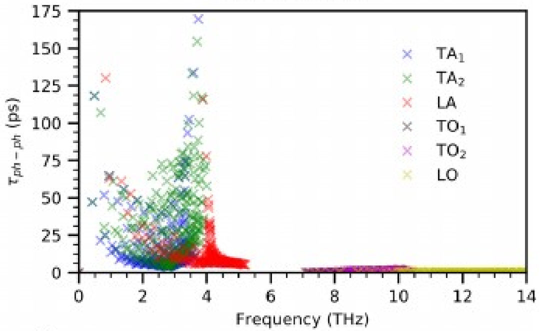


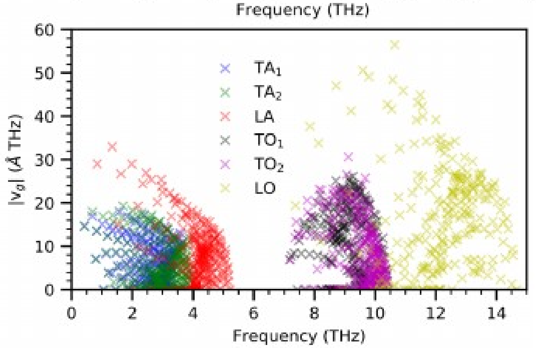


$$\frac{1}{\tau} = \frac{1}{\tau_{pd}} + \frac{1}{\tau_{ld}} + \frac{1}{\tau_{vd}} + \frac{1}{\tau_{gb}} + \frac{1}{\tau_{is}} + \frac{1}{\tau_{e-ph}} + \frac{1}{\tau_{ph-ph}}$$

$$\kappa_{ij} = \sum C v_i v_j \tau$$

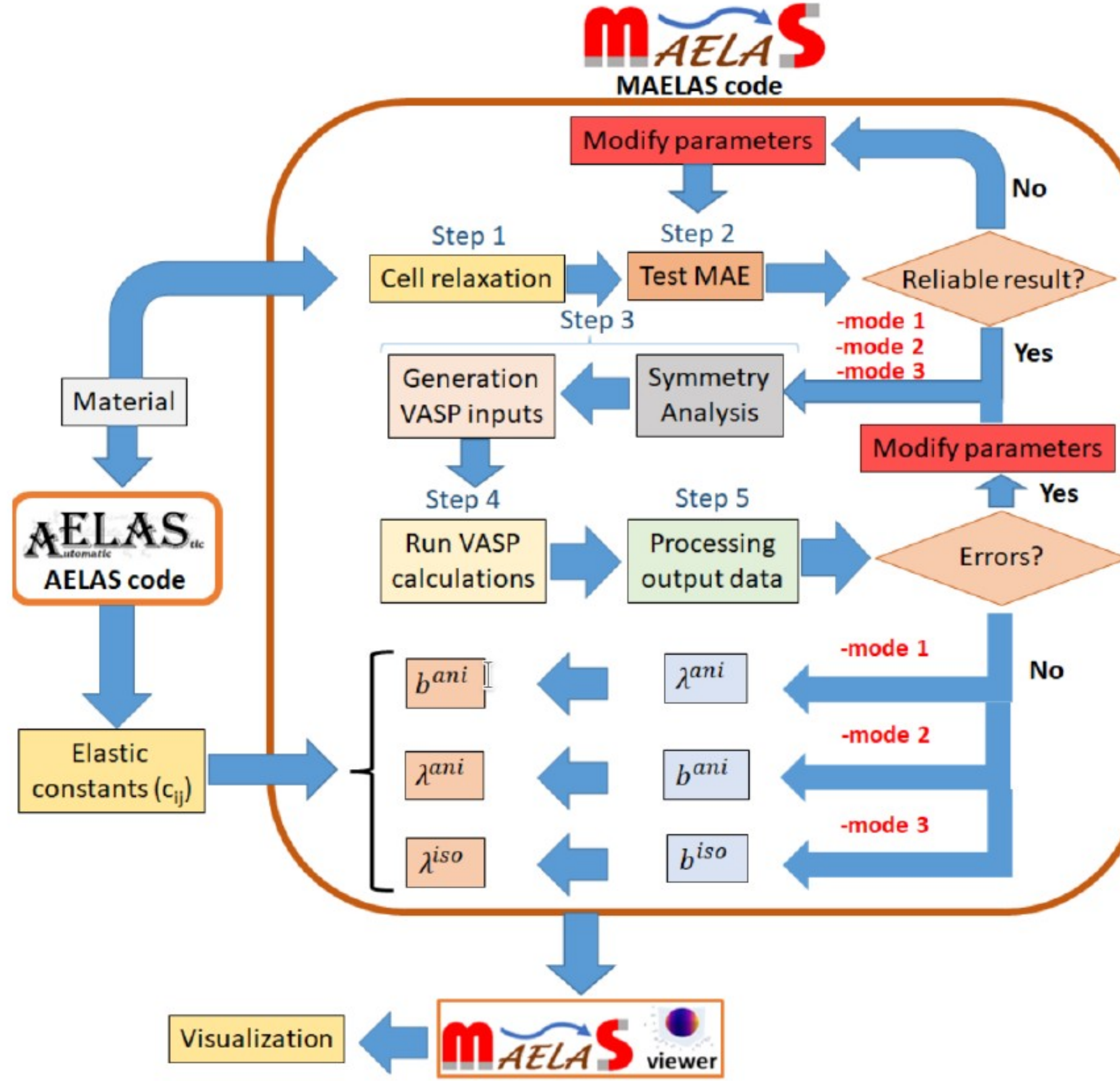






Material Design Towards Reality – www.md-esg.eu

Dr. Pablo Nieves – senior scientist - expert in multiscale modeling of magnetism – MAGNETOSTRICTION and MAGNETOELASTICITY



http://www.md-esg.eu/software/ http://www.md-esg.eu/maelasviewer/
Comp. Phys. Comm. **264**, 107964 (2021), Comp. Phys. Comm. **271**, 108197 (2022), Comp. Mat. Sci. **224**, 112158 (2023), Sensors **20**, 6436 (2020).

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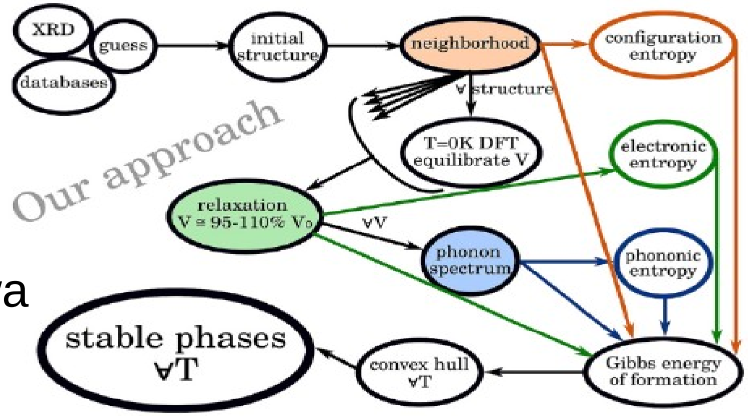
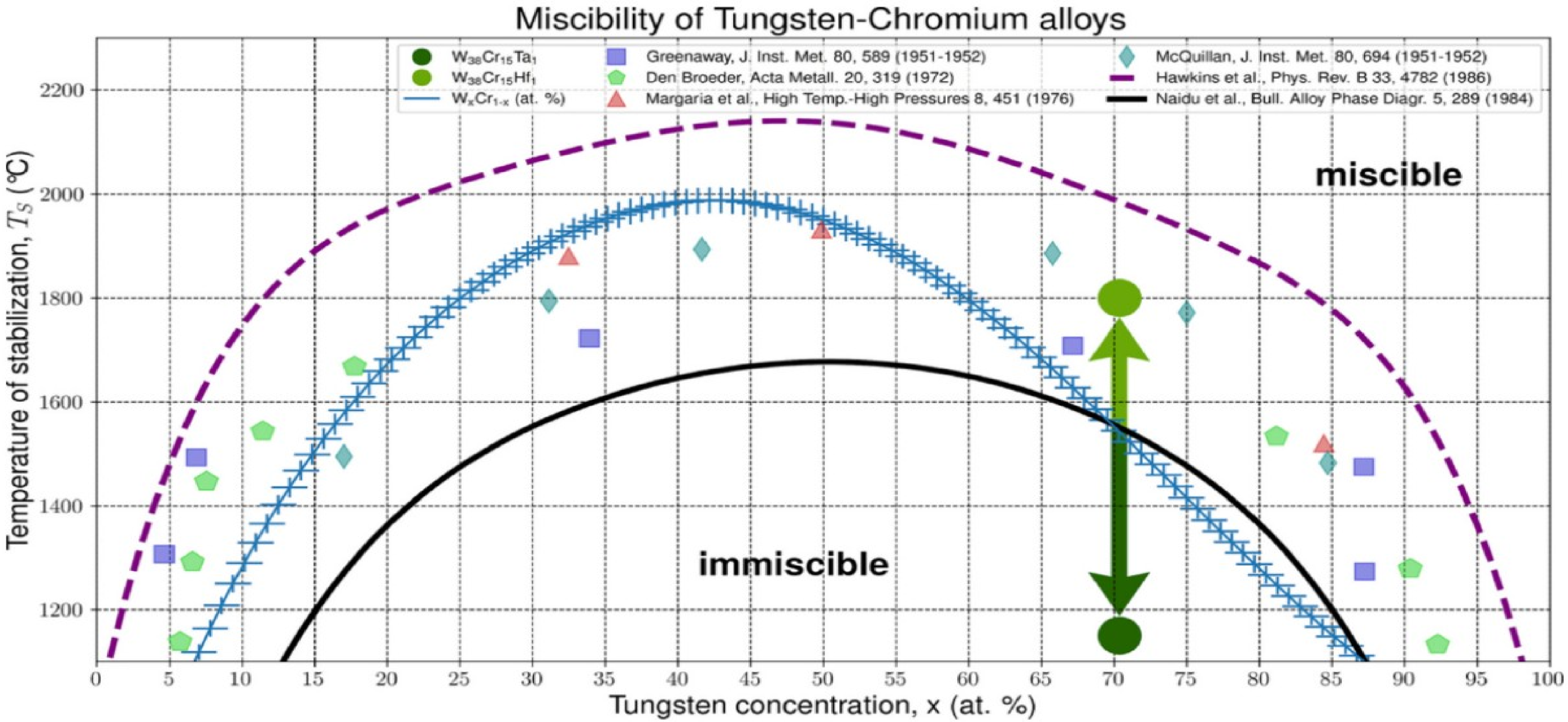
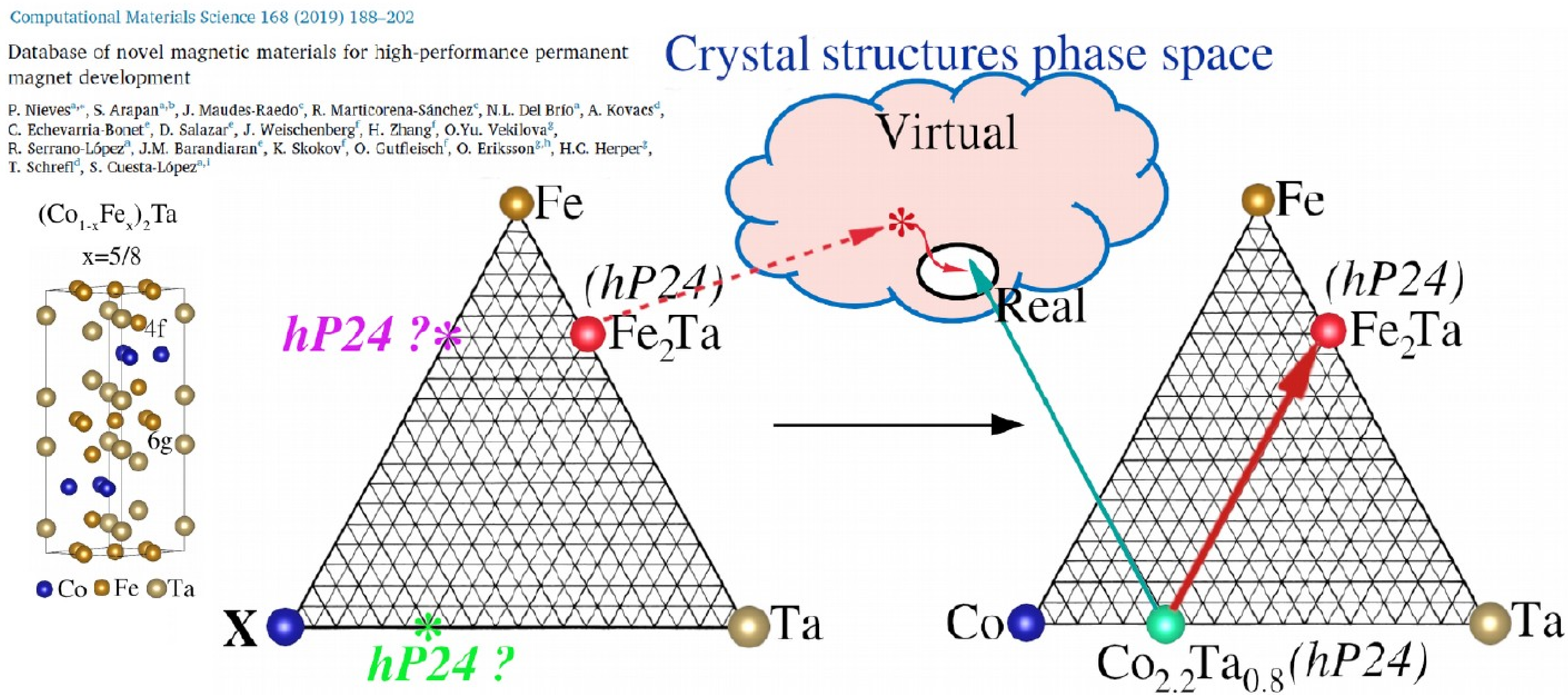
Dr. Andrzej Kadzielawa





Dr. Sergiu Arapan – senior scientist - expert in search for novel permanent magnets

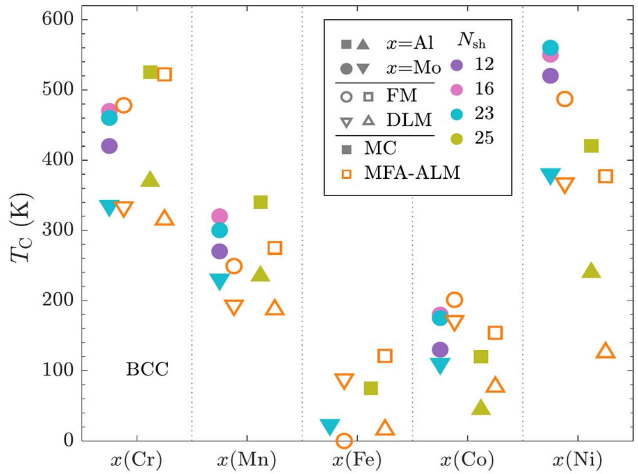


Phys. Rev. B **101**, 014426 (2020), Phys. Rev. Appl. (under review)

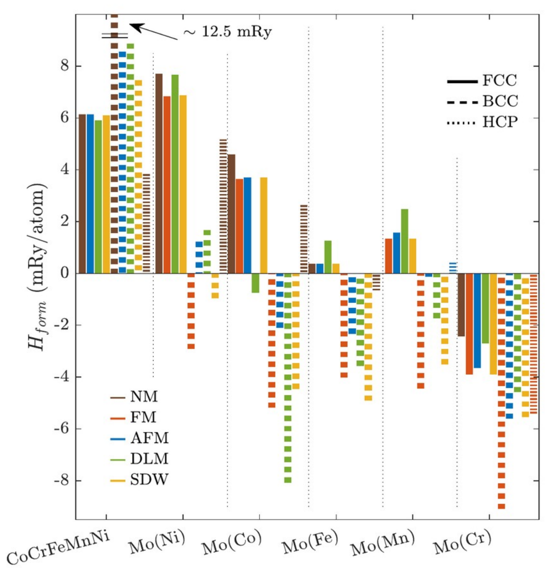
Material Design Towards Reality – www.md-esg.eu

Dr. Jakub Sebesta – junior scientist -
expert in chemical and magnetic disorder

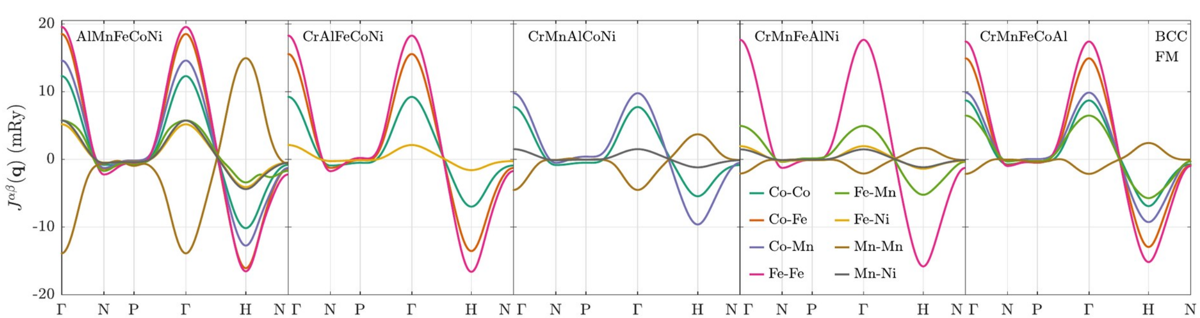
Material design
- 3*d* element based HEAs
- *p*, *d* non-magnetic substitutions
  CrMnFeCoNi non-magnetic
- composition × • stability • magnetic phase
  • mag. ordering temperature



- ferromagnetic ordering - importance of Fe, Co, Mn
  - leading exchange interaction
  - Fe essential for FM ordering
- substituted Cr, Ni atoms - stabilize FM state against the DLM one
- bcc structures
  × closed packed ones suppress magnetism
- T_C above room temperature achievable



JS, DL et. al., Phys. Rev. Mat. 3, 124410 / JS, DL et. al., Phys. Rev. B 103, 064407



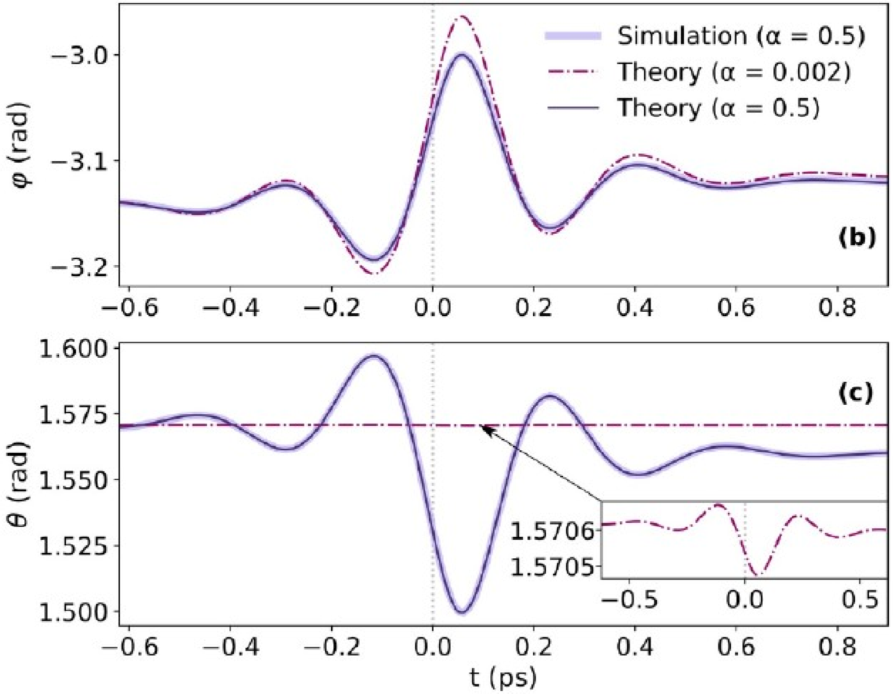
Dr. Ievgenia Korniienko – scientist - expert in spin dynamics modelling, detection of THz radiation – Zeeman torque

LLG eq.

$$\frac{\partial \mathbf{M}}{\partial t} = -\frac{\gamma}{1+\alpha^2}(\mathbf{M}\times\mathbf{H}) - \frac{\alpha\gamma}{M_s(1+\alpha^2)}\mathbf{M}\times(\mathbf{M}\times\mathbf{H})$$

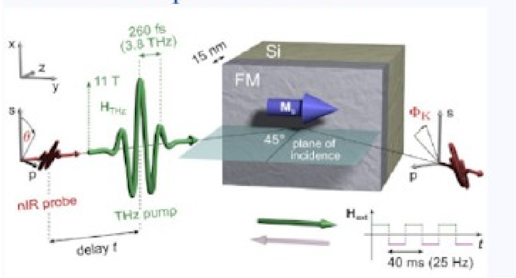
Precession of the magnetization

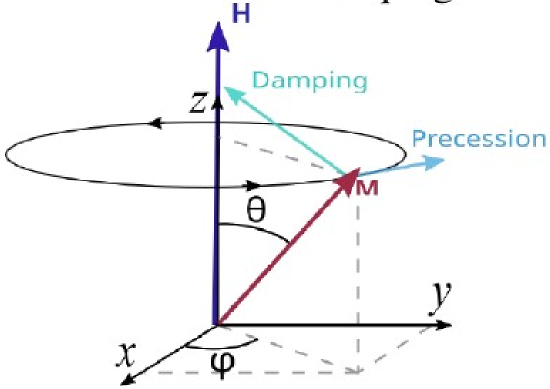
Damping



Phys. Rev. Applied (under review)

Available experimental data:



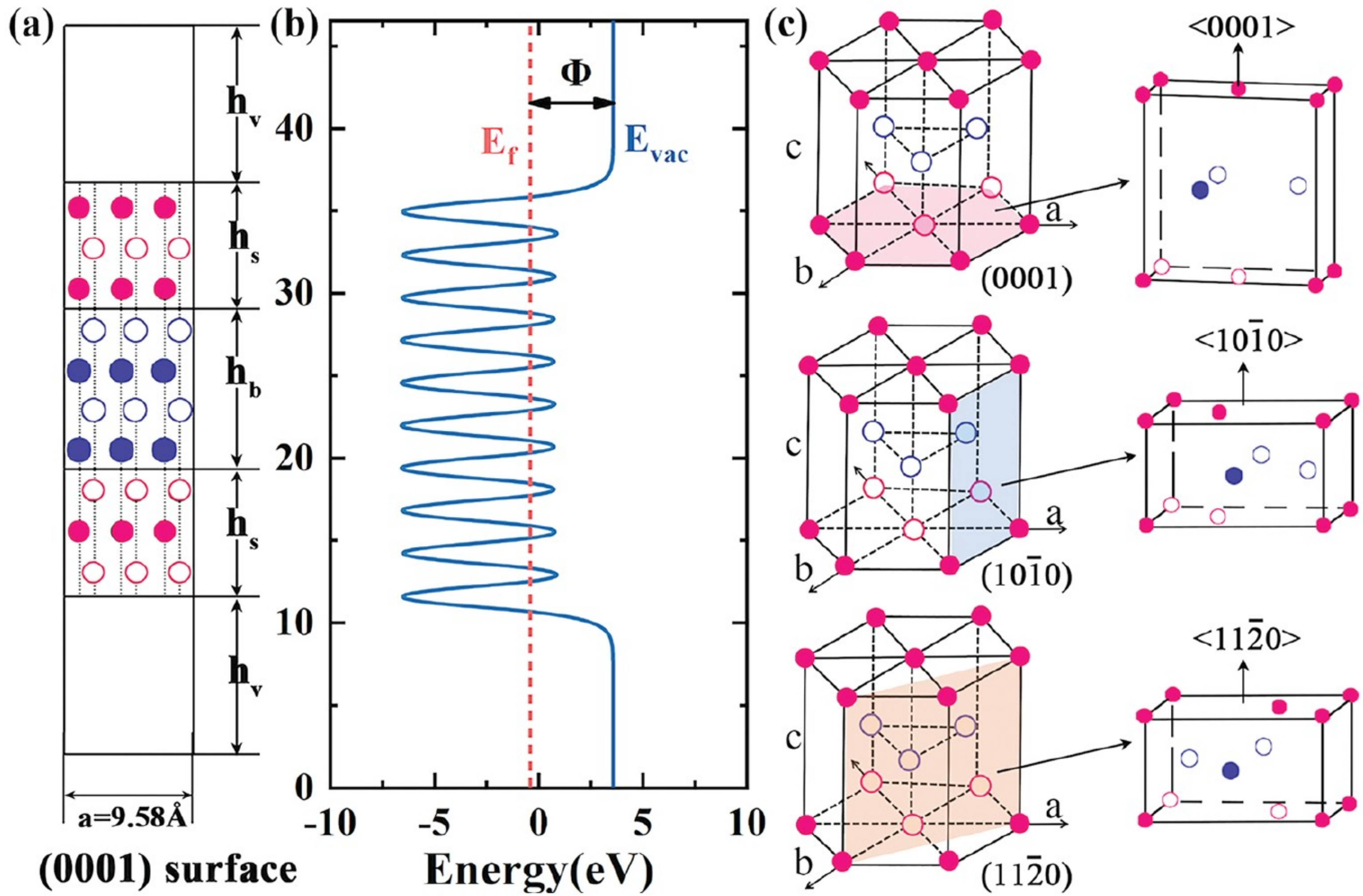


For small α ($\sim 10^{-3}$)
$\theta \approx$ const

Some Examples

Example 1. Polarization and surface energy vs strain

$$\gamma_s = \frac{E_s - nE_b}{2S}$$



Example: Polarization and surface energy vs strain

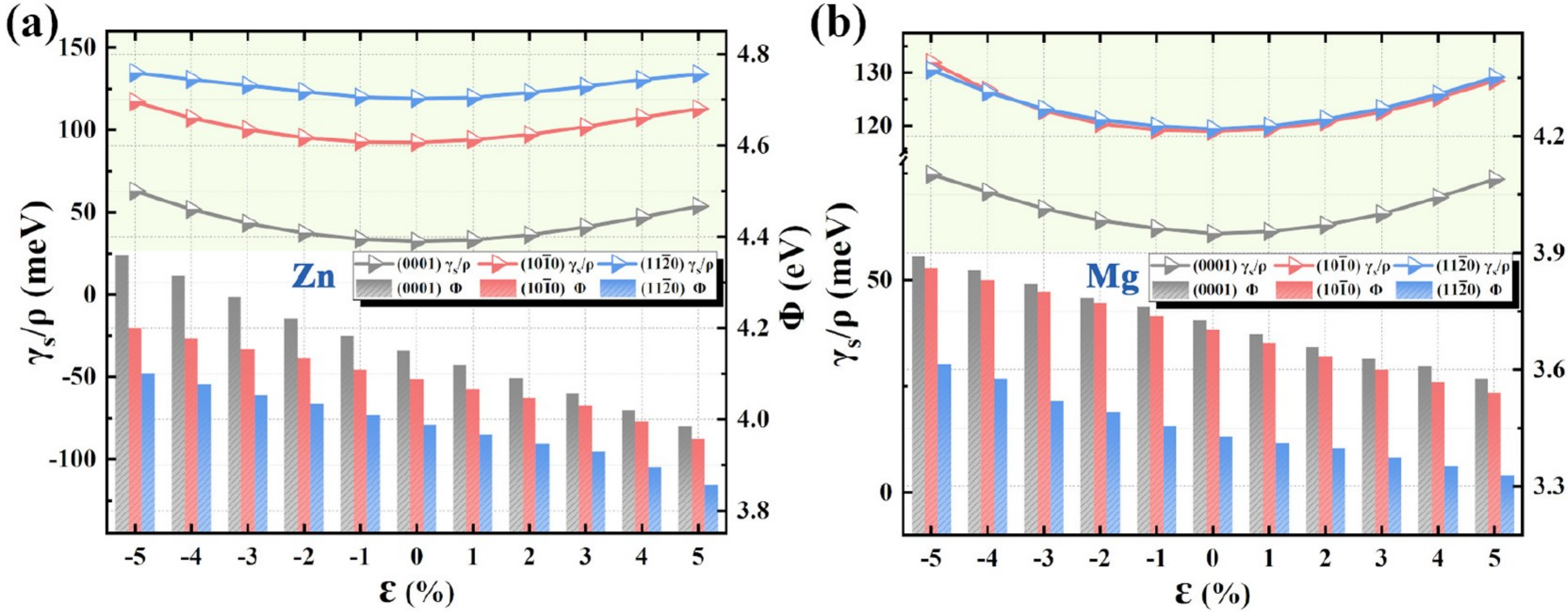
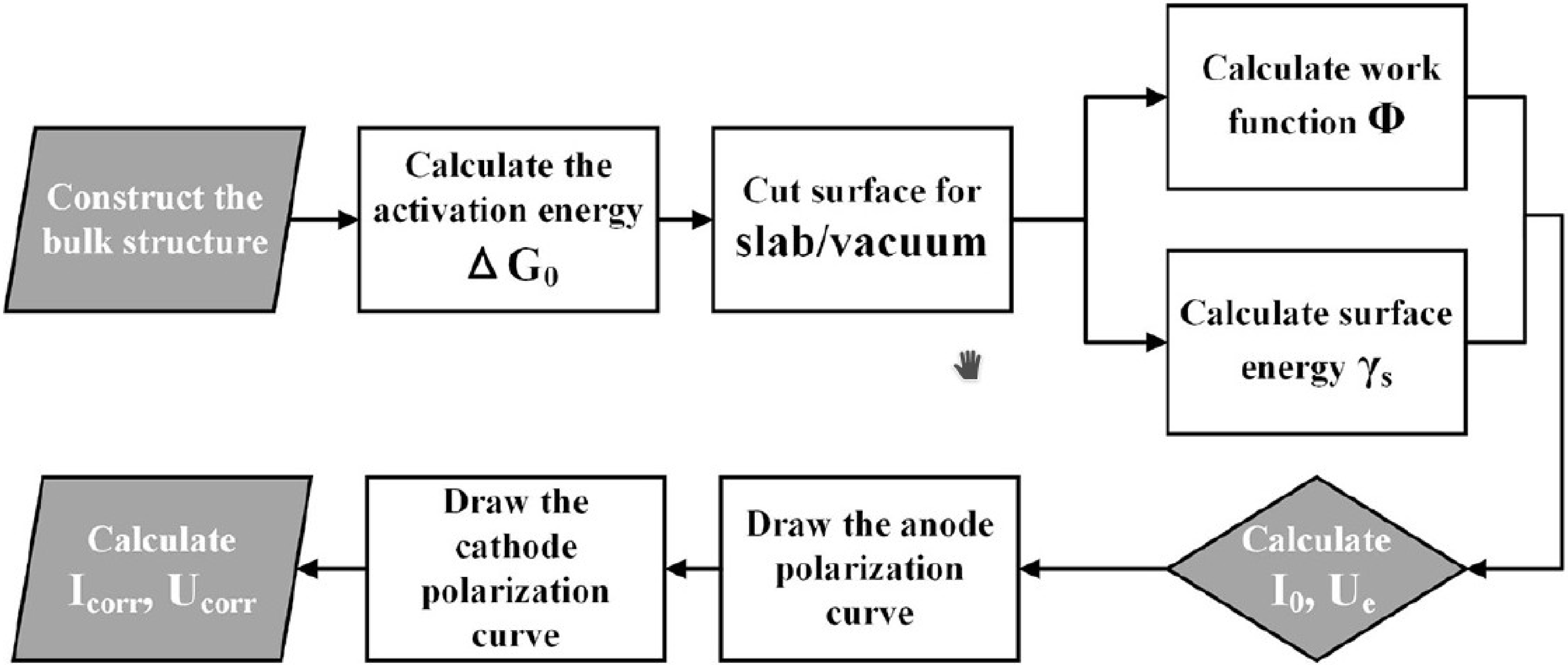
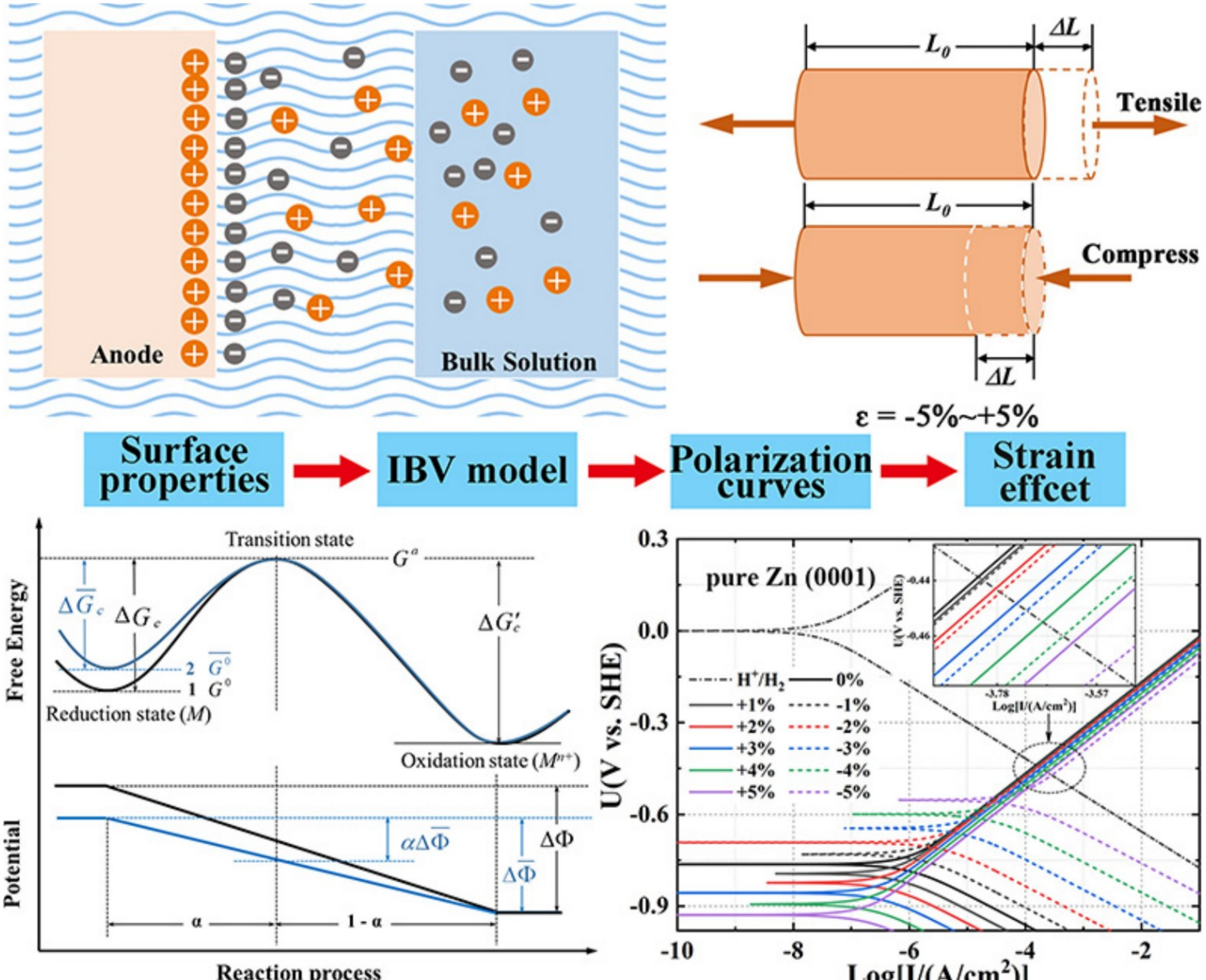


Fig. 2. The variations of surface energy density and work function vs. uniaxial strains (a) of pure Zn and (b) of pure Mg for the (0001), (10$\bar{1}$0) and (11$\bar{2}$0) surfaces.

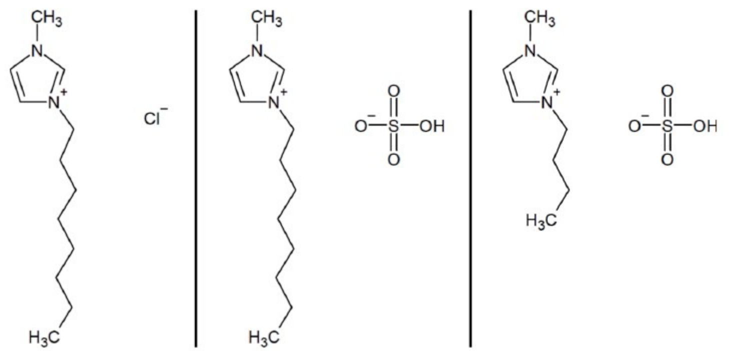
Example: Polarization and surface energy vs strain



Example: Polarization and surface energy vs strain



Example 2. Inhibition of corrosion



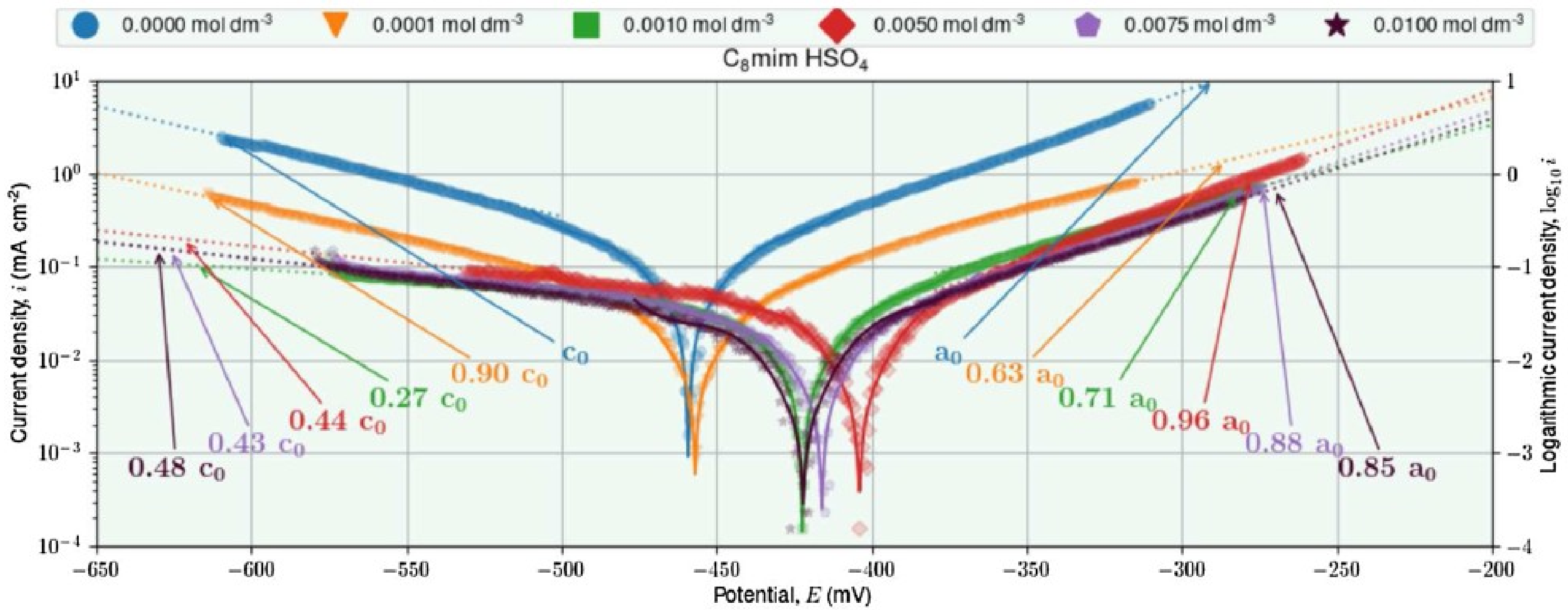
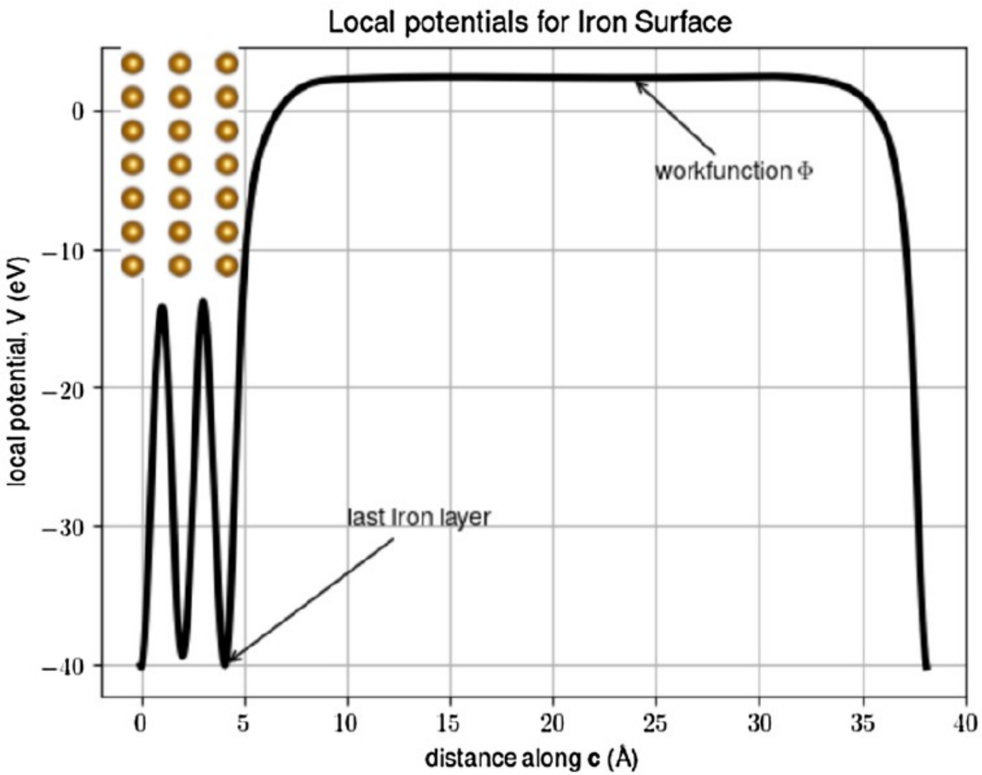
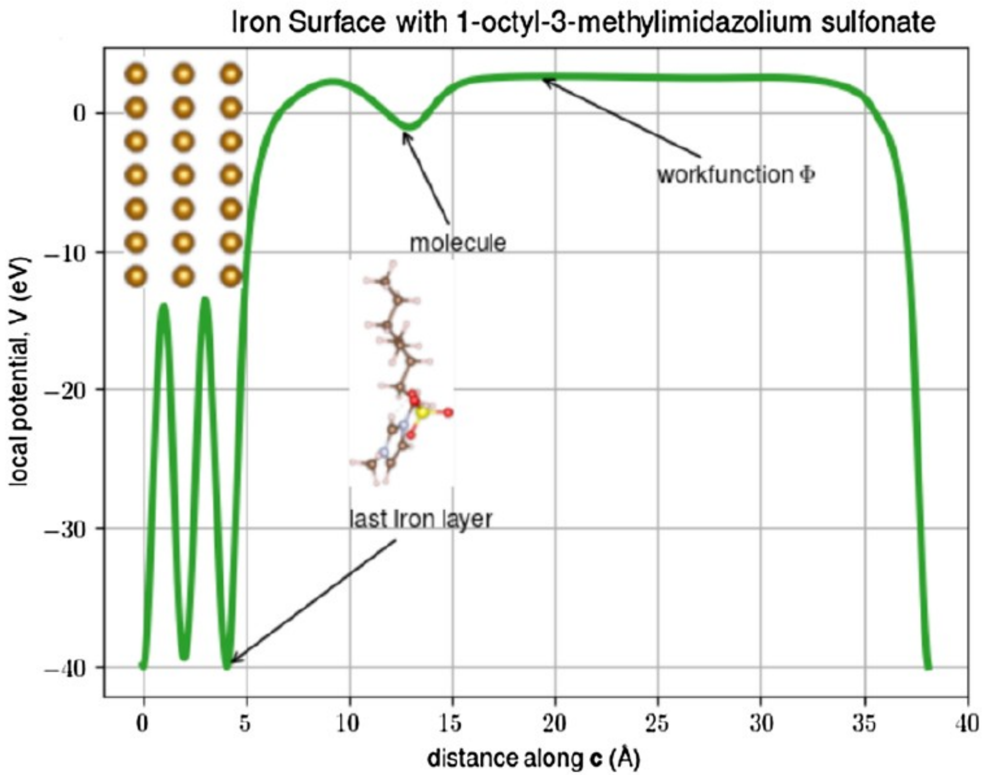


Fig. 3. Potentiodynamic polarization curves of corrosion inhibition of mild steel in 1 M HCl in the absence and presence of 1-octyl-3-methylimidazolium hydrogen sulphate. The numbers correspond to the ratio of the anodic (*a*) and cathodic (*c*) tails with respect to the values for a solution with no inhibitor (blue curve, a_0 and c_0). Solid lines are a guide to the eye. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Example – Inhibition of corrosion

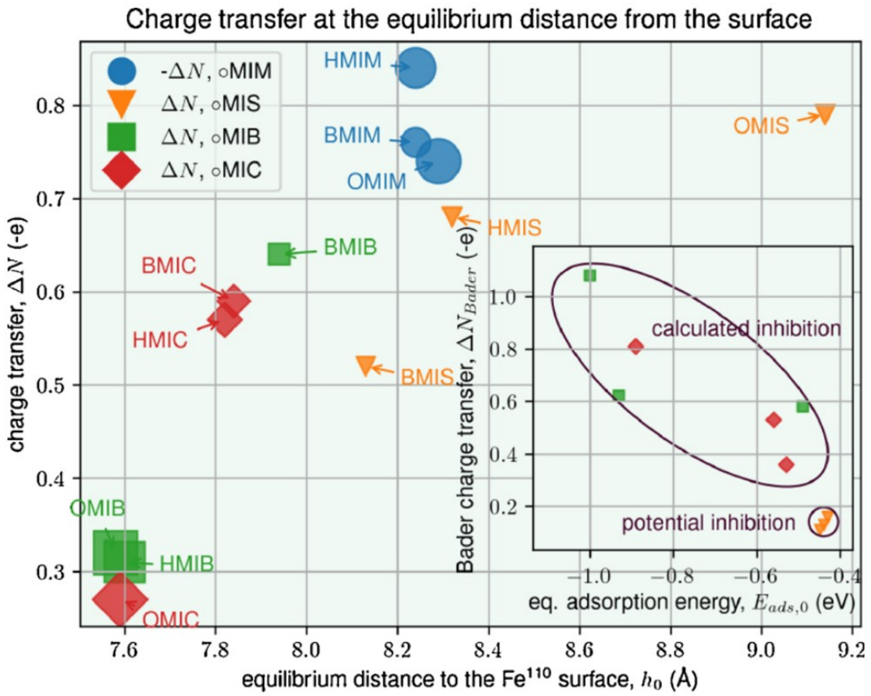




Example – Inhibition of corrosion

	E_{HOMO} on Fe(110)	E_{HOMO} free	E_{LUMO} on Fe(110)	E_{LUMO} free
BMIB	– 5.55	– 4.47	– 1.86	– 1.67
HMIB	– 6.48	– 4.52	– 1.75	– 1.67
OMIB	– 6.46	– 4.56	– 1.76	– 1.67
BMIC	– 5.70	– 4.70	– 1.77	– 1.49
HMIC	– 5.74	– 4.83	– 1.77	– 1.56
OMIC	– 6.66	– 4.81	– 1.74	– 1.55
BMIS	– 5.87	– 5.32	– 1.85	– 1.82
HMIS	– 5.60	– 5.37	– 1.81	– 1.86
OMIS	– 5.46	– 5.39	– 1.72	– 1.82

	η (eV) on Fe(110)	η (eV) free	χ (eV) on Fe(110)	χ (eV) free	ΔN on Fe (110)	ΔN free
BMIB	1.84	1.40	3.71	3.07	0.64	0.21
HMIB	2.36	1.42	4.12	3.10	0.31	0.22
OMIB	2.35	1.44	4.11	3.11	0.32	0.22
BMIC	1.97	1.60	3.73	3.09	0.59	0.20
HMIC	1.98	1.63	3.75	3.19	0.57	0.22
OMIC	2.46	1.64	4.20	3.19	0.27	0.22
BMIS	2.01	1.75	3.86	3.57	0.52	0.31
HMIS	1.89	1.76	3.70	3.61	0.68	0.32
OMIS	1.87	1.79	3.59	3.62	0.79	0.32



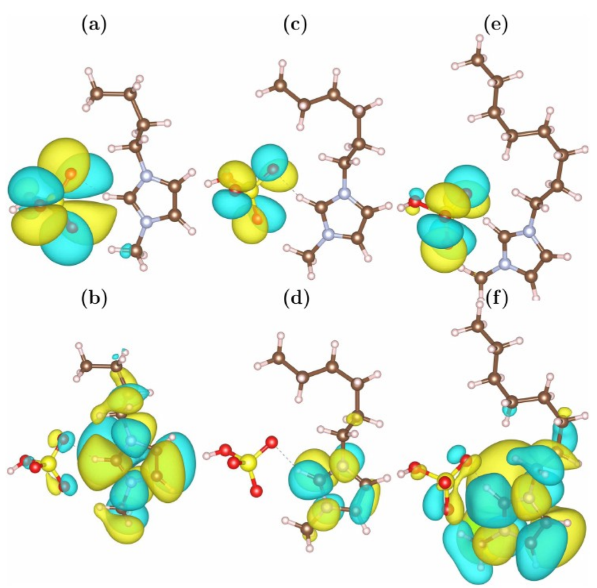
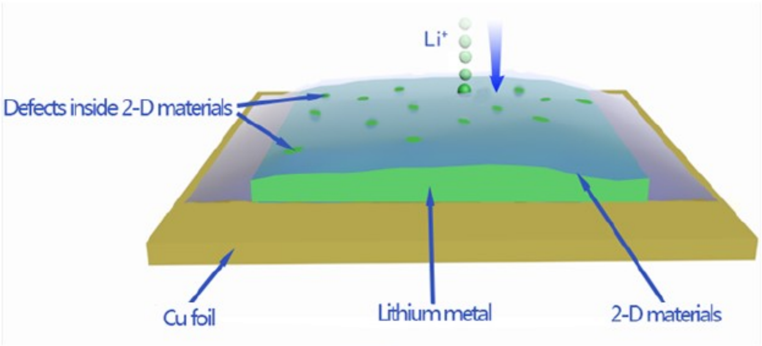


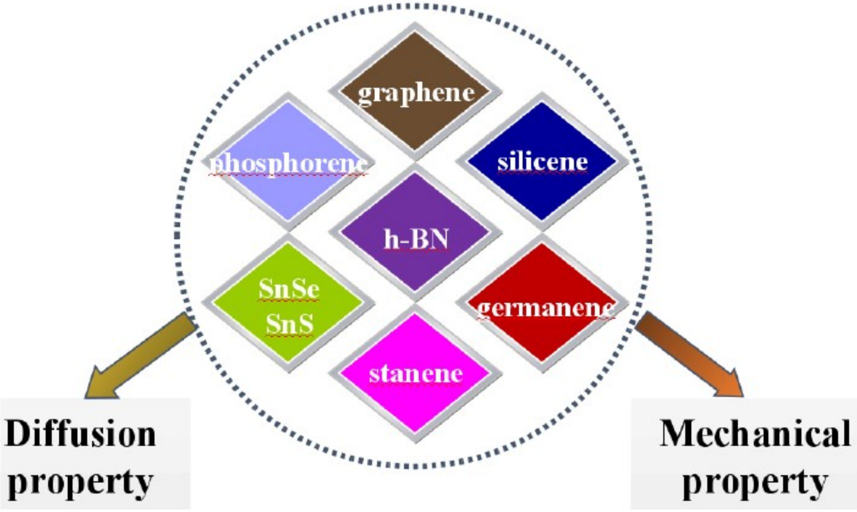
Fig. 18. The highest occupied molecular orbital (HOMO) (**top**) and the lowest unoccupied molecular orbital (LUMO) (**bottom**) wavefunctions of 1-butyl-3-methylimidazolium hydrogen sulphate **(a), (b)**; 1-hexyl-3-methylimidazolium hydrogen sulphate **(c), (d)**; 1-octyl-3-methylimidazolium hydrogen sulphate **(e), (f)**.

Example – 2D materials - Diffusion

Different layered structure materials
- influenced by:

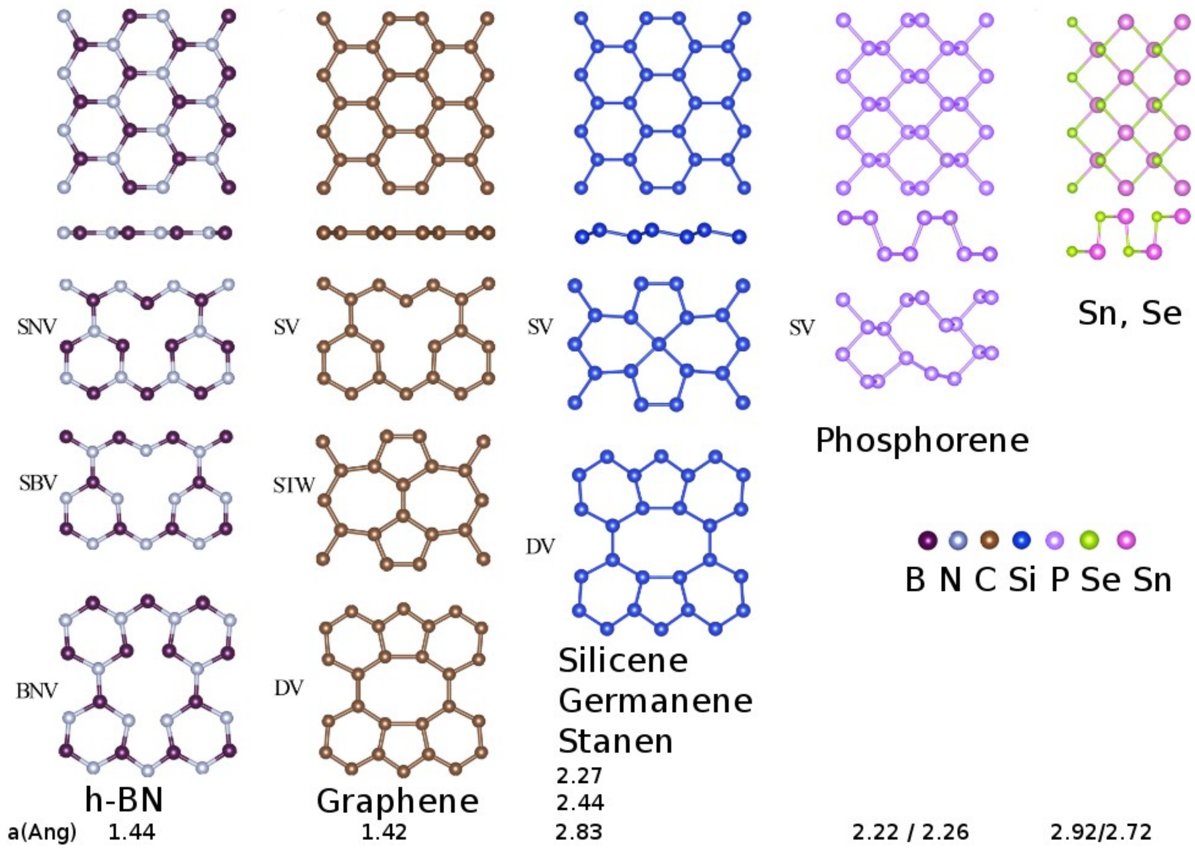
- crystalline structure
- defect
- metal proximity



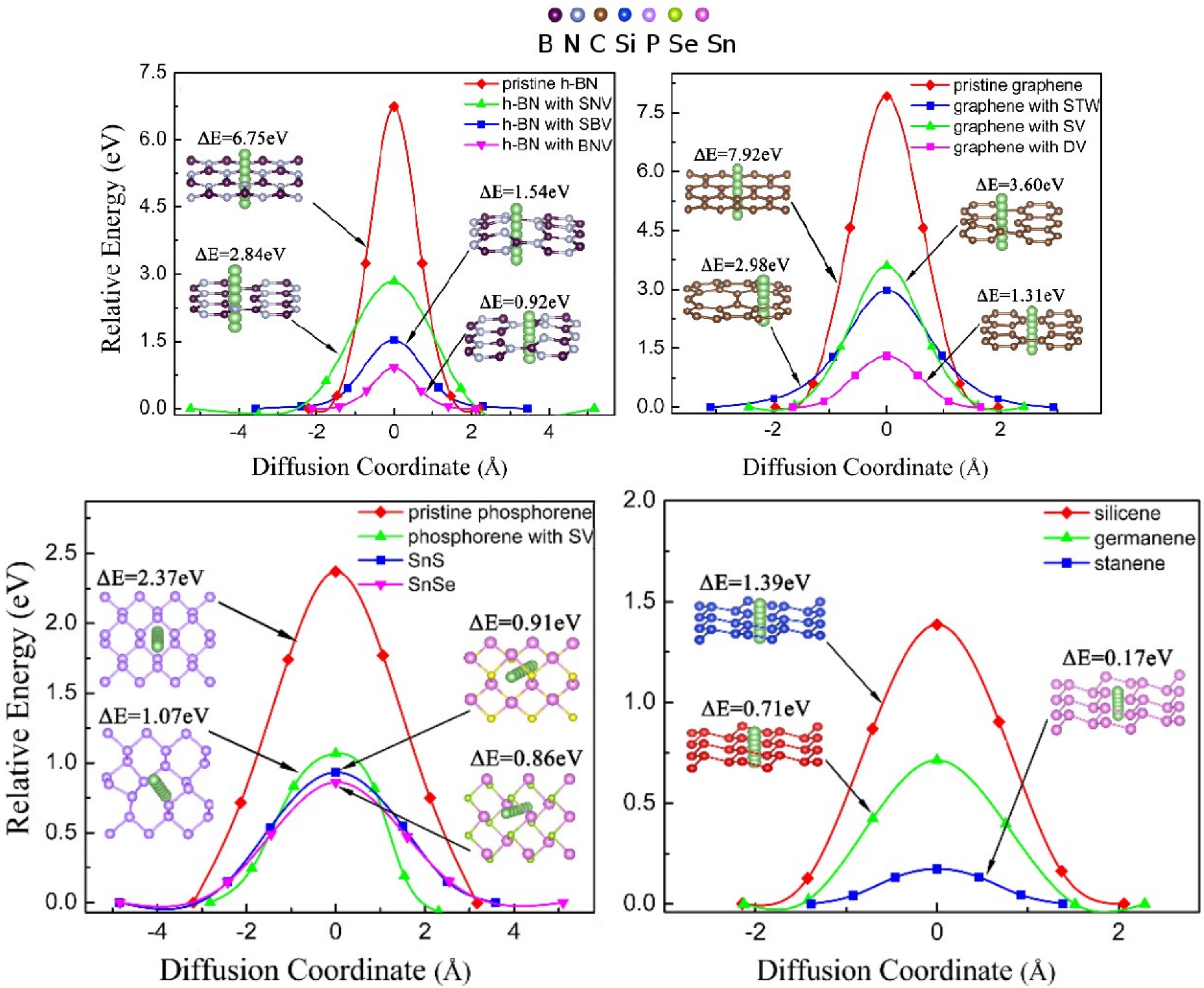


$$D = l^2 \upsilon^{\frac{-\Delta E}{k_B T}}$$

$$l\text{..migr. dist.}, \ \upsilon = \left(\frac{2\Delta E}{ml^2}\right)^{\left(\frac{1}{2}\right)}$$

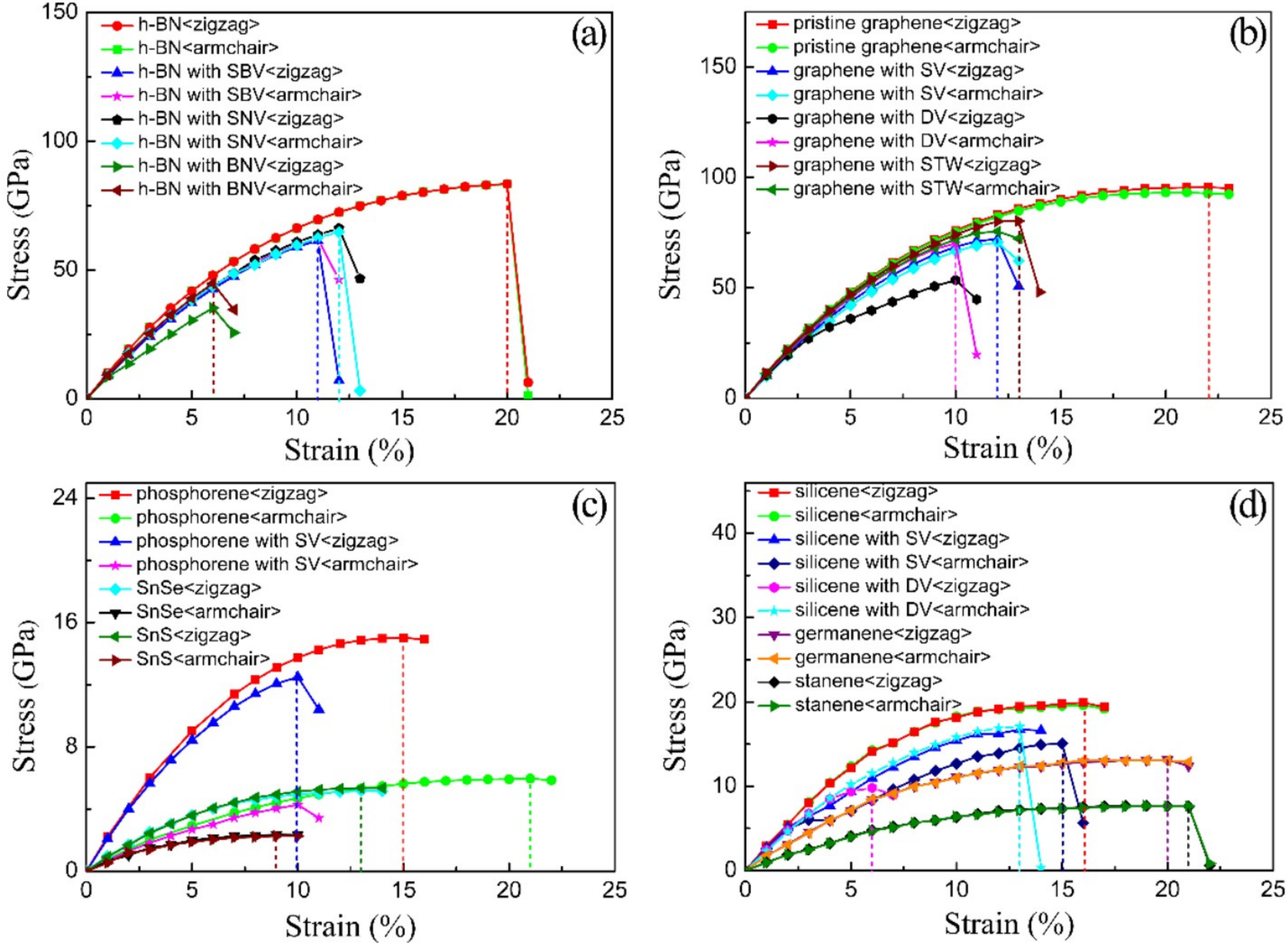


Example – 2D materials - Diffusion



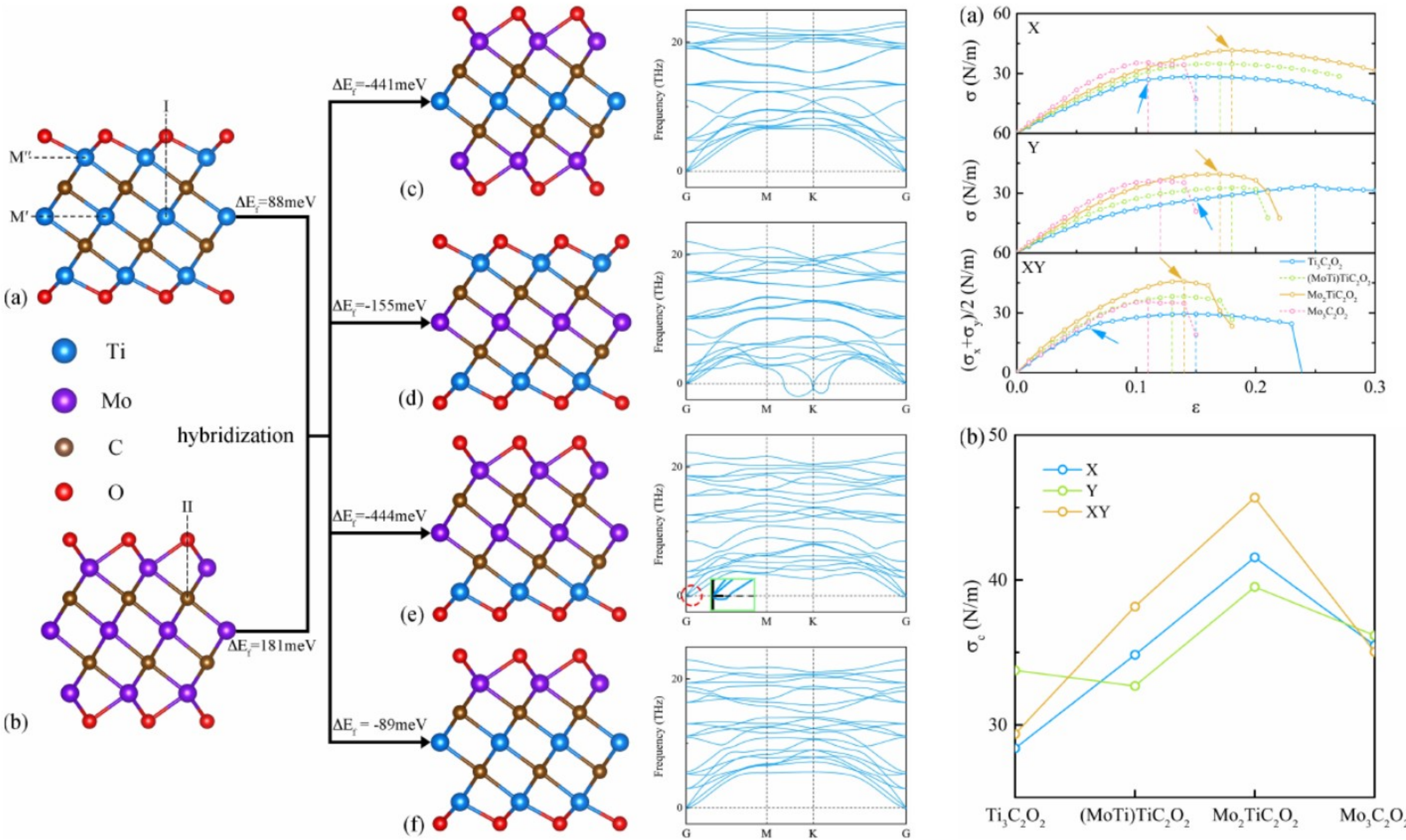
Affected by bond legnth, crystalline structure, and vacancy type

Example – 2D materials – Mechanical properties



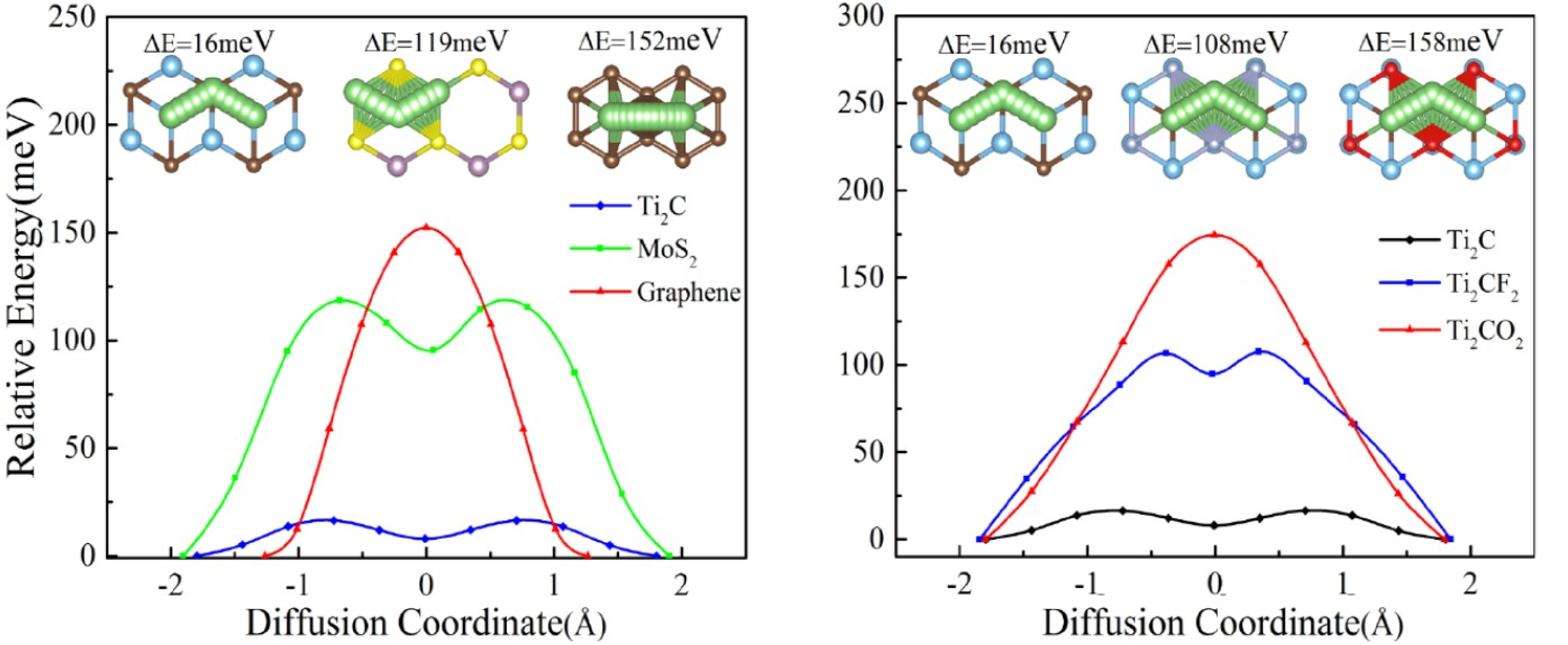
Defect can greatly weaken the strength of protective materials.

Example – 2D materials – Stability of Mxenes



Based on different instability modes in Ti_2CO_2 and Mo_2CO_2, we can build a hybrid MXenes. We can get a higher ideal strength than the pure substances.

Example – 2D materials – Diffusion at Mxenes surfaces



bare MXenes > graphene, MoS_2 and functionalized MXenes

The increasing barriers is attributed to strong chemical bonds between surface groups and Li ions

PNAS **114**, E110827 (2017)

Introductory remarks

The course concerns “Theoretical aspects of surface physics”

- Few examples out of vast number will be given

- Lecture will also address some computational methods, but basically their main principles, pros & cons, with emphasis on physical problems rather than technicalities
- > suited for experimentalists

- Indeed, this is an idea of the exam’s essay, that in such might be useful for both you and us

Introductory remarks – time-schedule of lectures

Introduction to theoretical surface physics

Faculty of Mathematics and Physics, Trója
Friday, room 320, third floor (seminar room of Department of Surface and Plasma Science)
10:40 - 12:10

Dominik Legut (DL)
Ondřej Šipr (OS)

13. 10. DL: Introduction and examples of solid surfaces phenomena

20. 10. OS: Electronic structure of solids - basic concepts

27. 10. OS:Electronic structure of surfaces

3. 11. DL: Surface structure and its investigation by experiment and theory

10. 11. DL: Chemisorption I. - basic concepts and models

24. 11. OS: Density functional theory

1. 12. DL: Chemisorption II. - realistic examples

8. 12. OS: Photoemission spectroscopy

15. 12. OS: Core level spectroscopy: XES, XAS, PED

22. 12. DL: Surface-related calculations: a practical session

5. 1. DL: Inhibition, diffusion, and catalytic perfomance on surfaces

12. 1. OS: Magnetism of surfaces

16. 1. (Tuesday) ***Deadline for submitting the examination essays***

26. 1. 10:00 *Examination seminar (first group of students)*

2. 2. 10:00 *Examination seminar (second group of students)*