Autonomous Workflows for an Accelerated Design of 1D Nanostructures and Battery Electrodes

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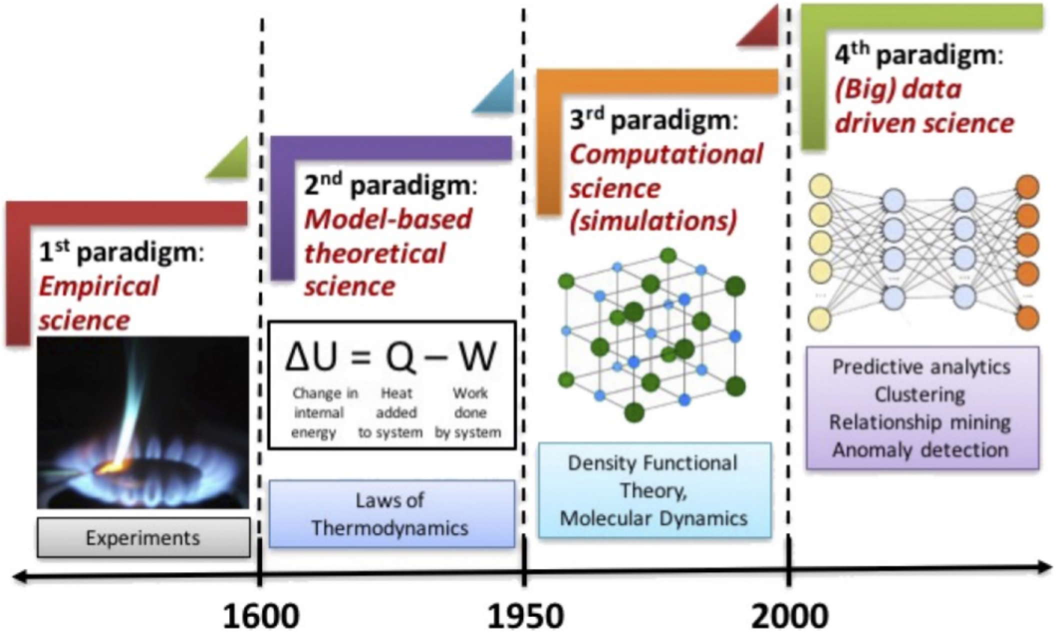
Department of Energy Conversion and Storage (DTU Energy)
Technical University of Denmark

Challenges for Sustainable Development

To solve many of these issues, we need to discover novel materials

Materials Discovery – A Bit of History

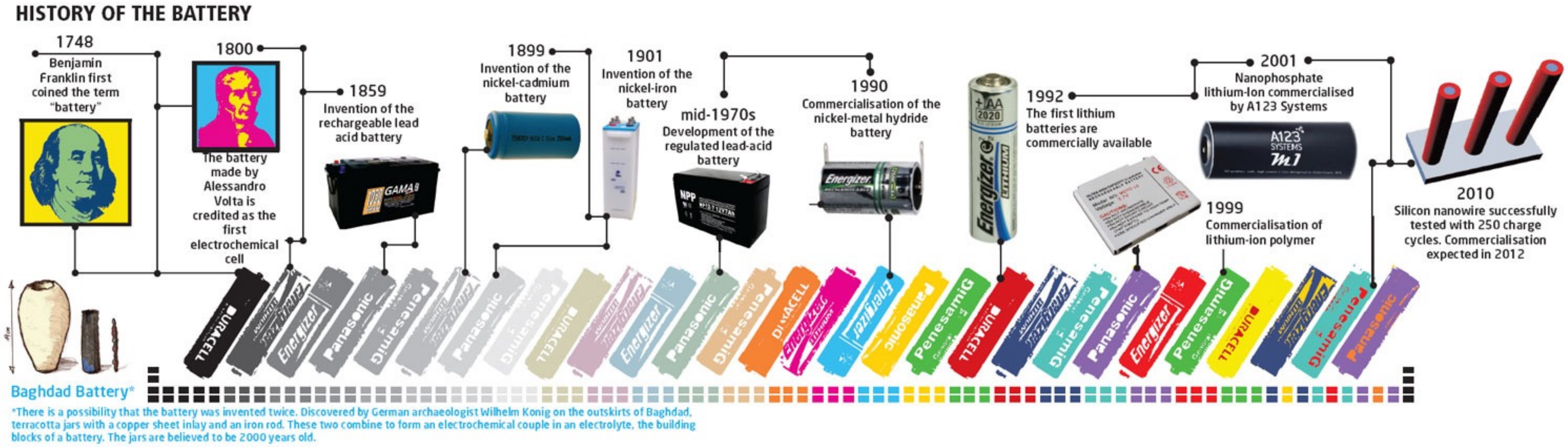


Angrawal and Choudhary, APL Materials 4, 053208 (2016)

Jose and Ramakrishna, Applied Materials Today 10, 127 (2018)

https://www.upsbatterycenter.com

Pancorbo, DOI: 10.13140/RG.2.2.14706.04806 (2018)



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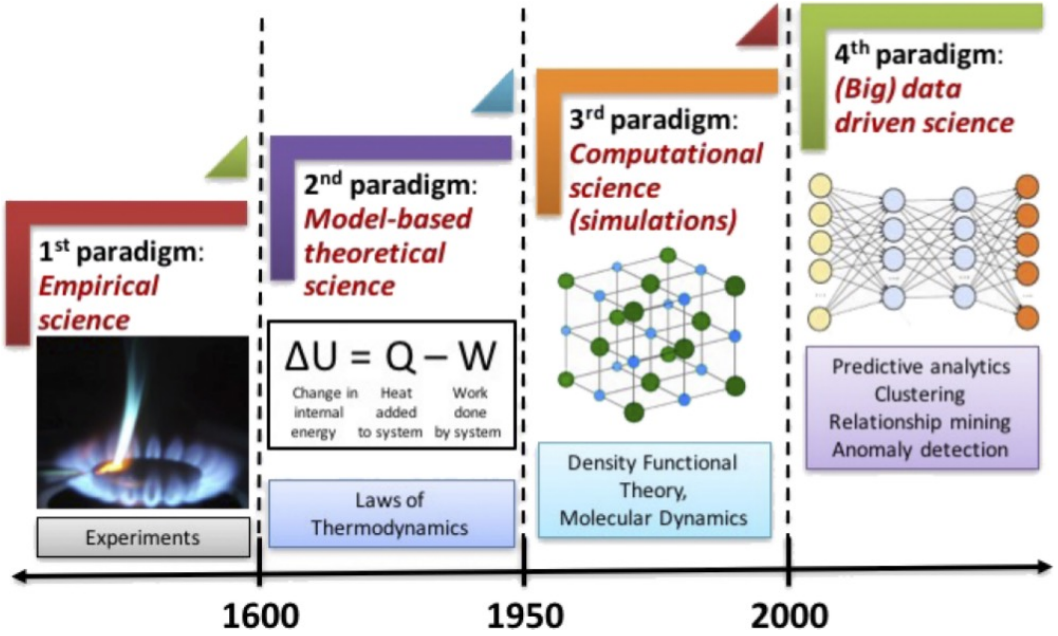

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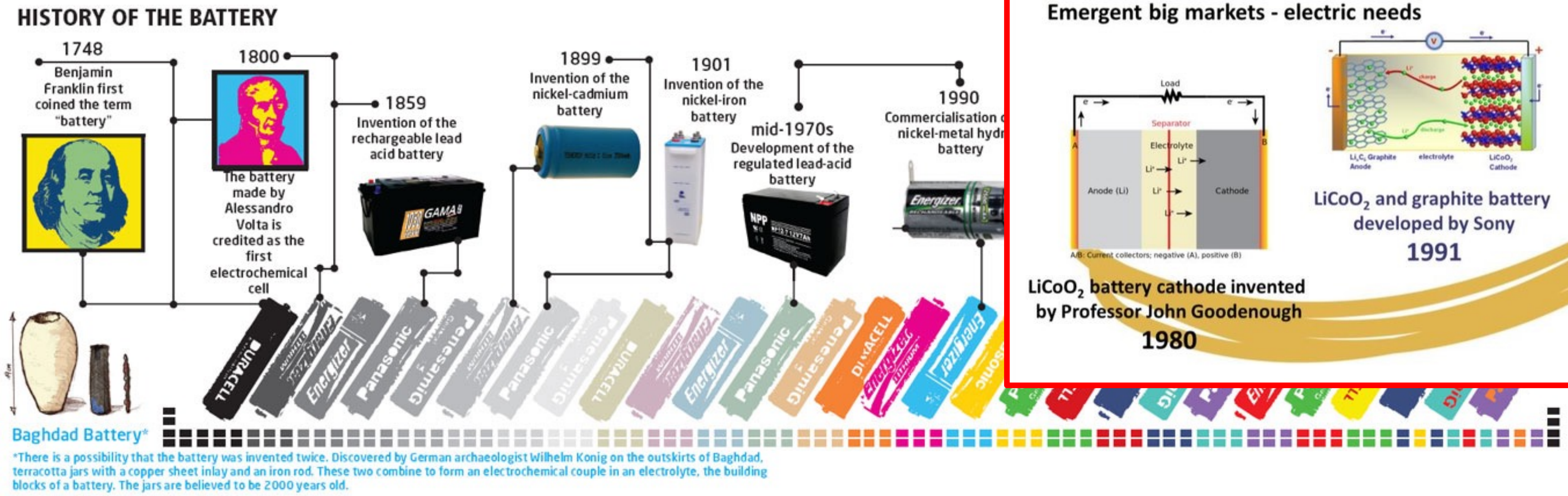
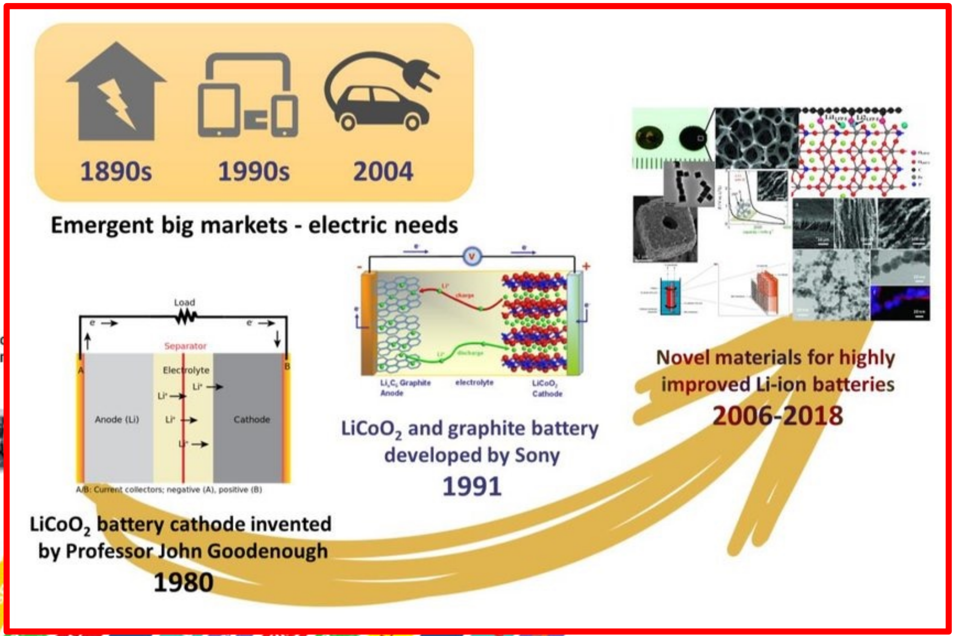
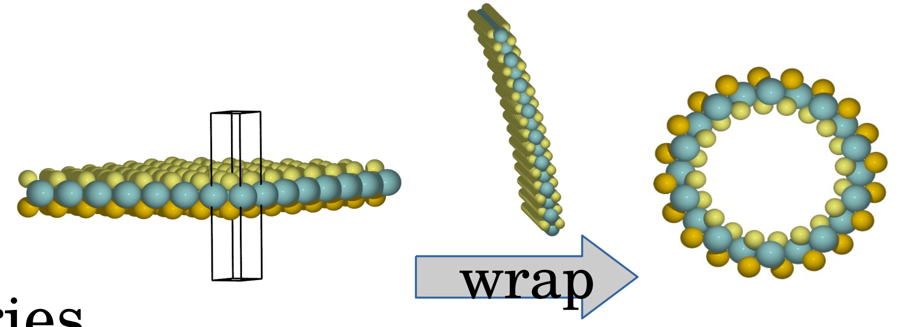




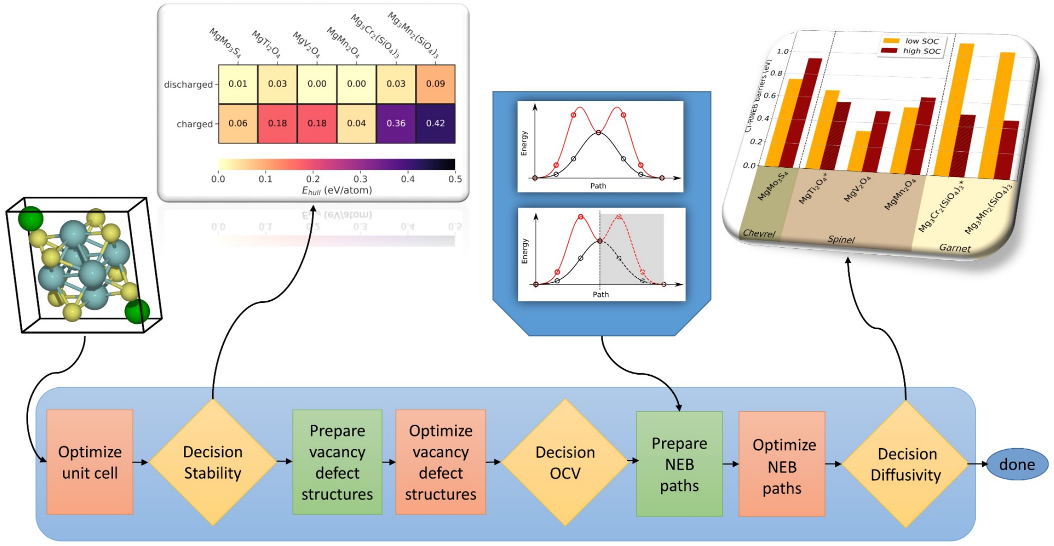
Autonomous Workflows for Materials Discovery – Outline

1) From 2D sheets to 1D inorganic nanotubes

Vision: use shape as a new degree of freedom to discover new materials

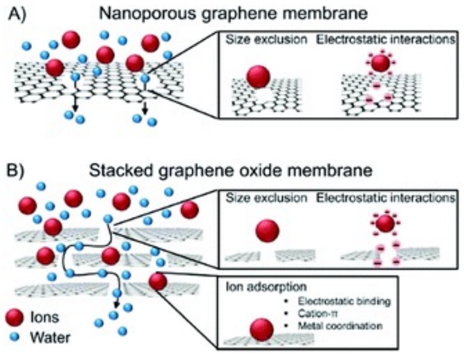


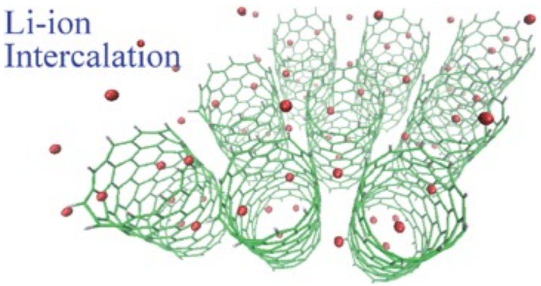
2) New electrodes for intercalation secondary batteries



3) Workflows for interfaces – is it a dream?

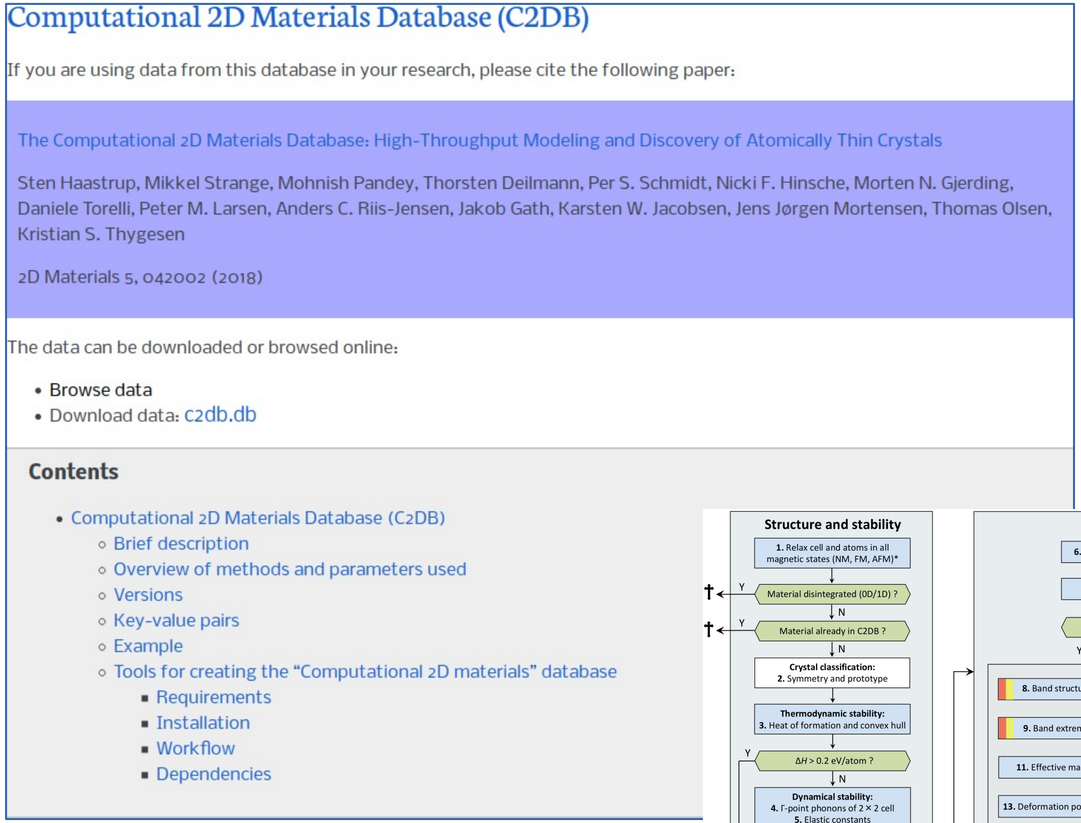
From 2D Databases to Inorganic 1D Nanotubes





Possible applications:

- water filtration/membranes
- anode materials for batteries
- catalysts
- health (drug delivery)
- nanofriction
- electronics
- magnetic effects



Computational 2D Materials Database (C2DB)

If you are using data from this database in your research, please cite the following paper:

The Computational 2D Materials Database: High-Throughput Modeling and Discovery of Atomically Thin Crystals

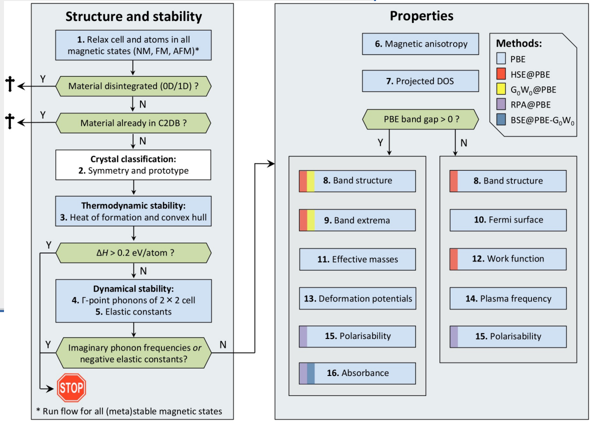
Sten Haastrup, Mikkel Strange, Mohnish Pandey, Thorsten Deilmann, Per S. Schmidt, Nicki F. Hinsche, Morten N. Gjerding, Daniele Torelli, Peter M. Larsen, Anders C. Riis-Jensen, Jakob Gath, Karsten W. Jacobsen, Jens Jørgen Mortensen, Thomas Olsen, Kristian S. Thygesen

2D Materials 5, 042002 (2018)

The data can be downloaded or browsed online:

- Browse data
- Download data: c2db.db

Contents



Dervin, Dionysiou and Pillai, *Nanoscale* **8**, 15115 (2016)

Santhosh, Nivetha, Kollu, Srivastava, Sillanpää, Grace and Bhatnagar, *Scientific Reports* **7**, 14107 (2017)

Song, Yang, Zhao and Fang, *Energy & Environmental Science* **4**, 1379 (2011)

Panchakarla and Tenne, *Nanotechnology for Energy Sustainability* 745 (2017)

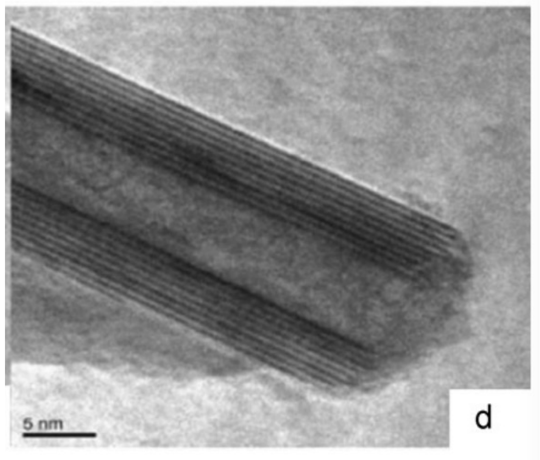
Haastrup, …, and Thygesen, *2D Materials* **5**, 042002 (2018)

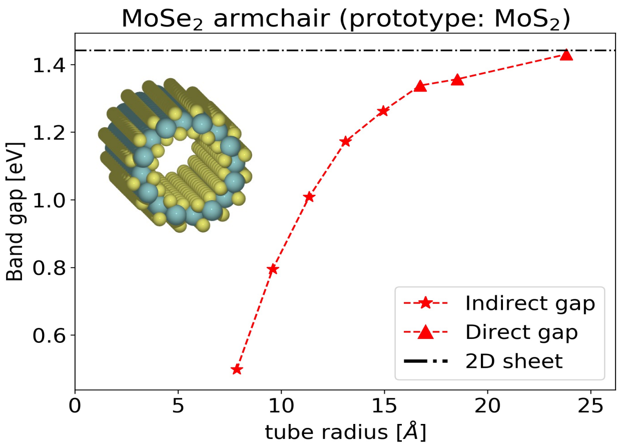
https://cmr.fysik.dtu.dk/c2db/c2db.html

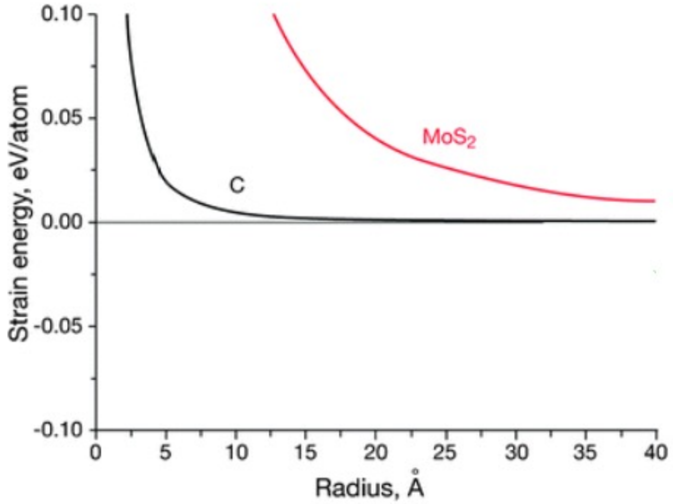
Inorganic Janus Nanotubes

Most inorganic nanotubes are multiwalled → no preferred size, difficult to tune properties

Inorganic single walled exists, **but** have large radii (> 35 Å) with properties close to the 2D limit







Seifert, Köhler, and Tenne, *J. Phys. Chem. B* **106**, 2497 (2002)

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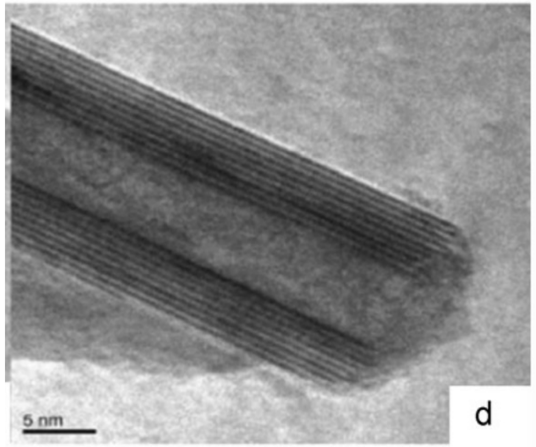

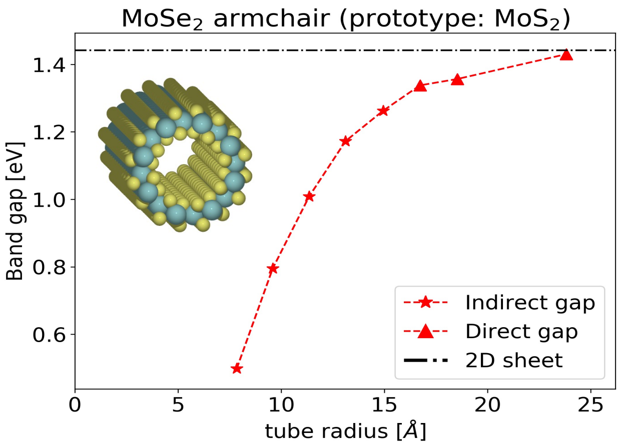

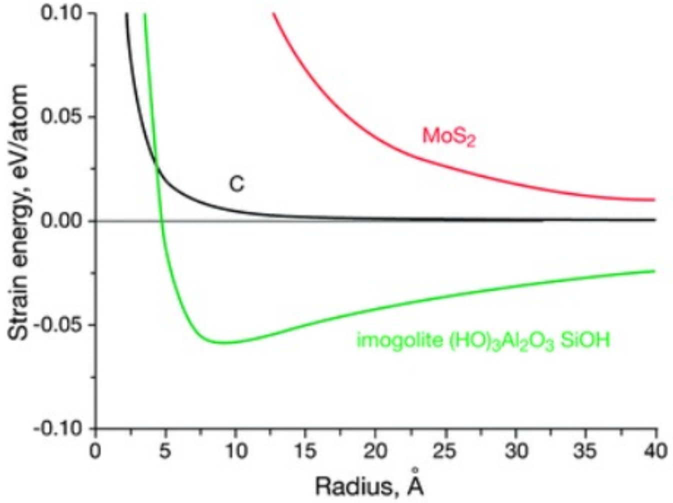

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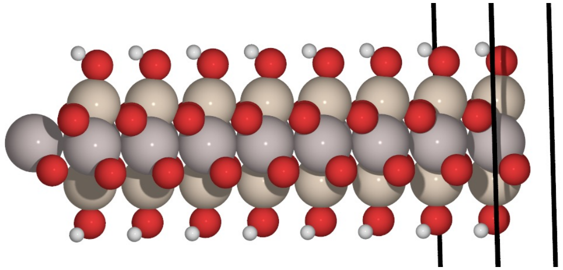
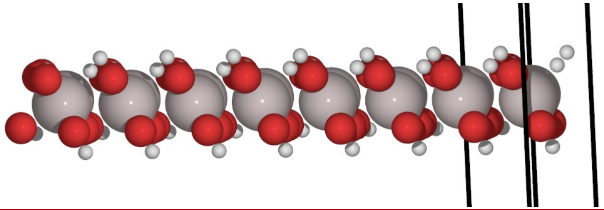
1st Janus Nanotube: Imogolite



$Al_2O_6(SiOH)_2$
a = 4.8 Å



$Al_2O_6(H_3)_2$
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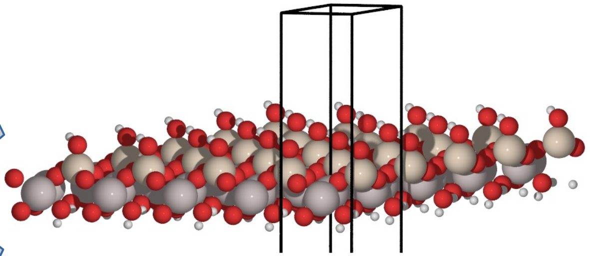
H_3 | $\mathbf{O_3Al_2O_3}$ | SiOH



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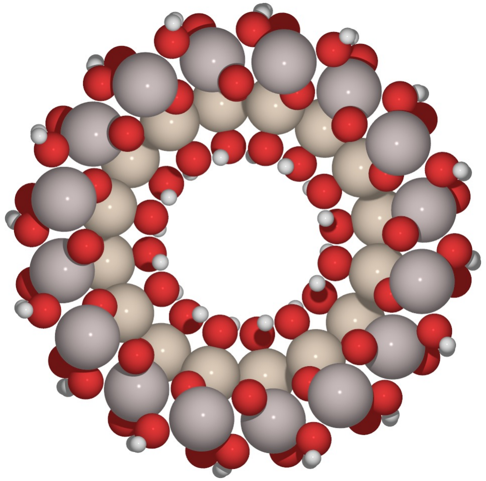

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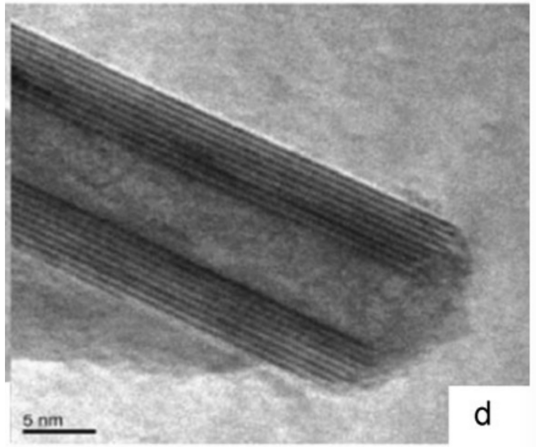

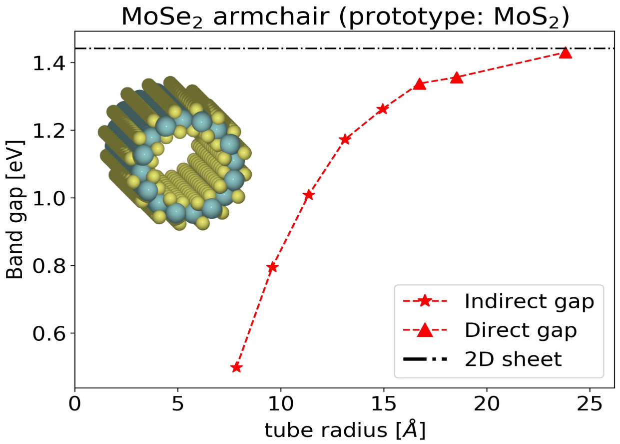

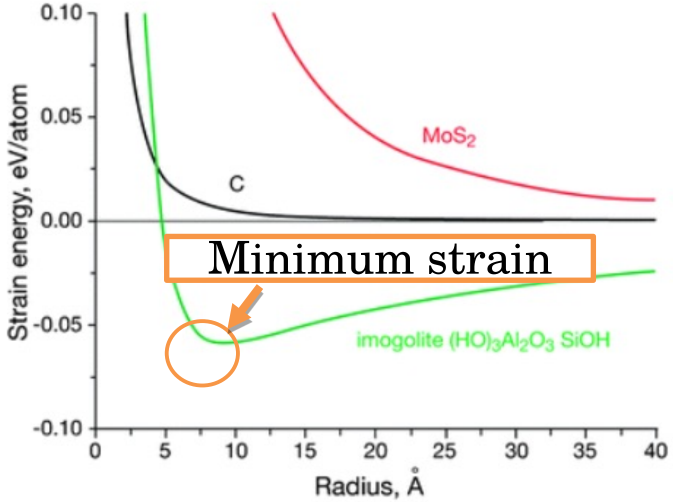

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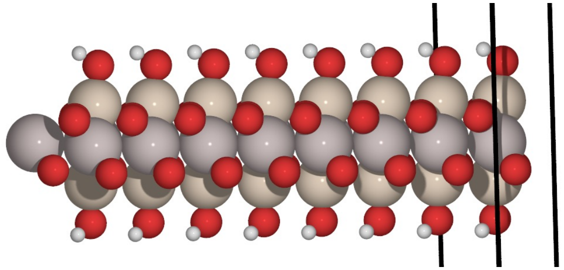

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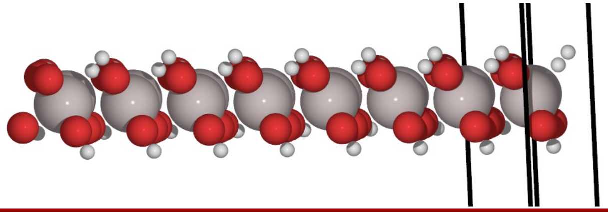

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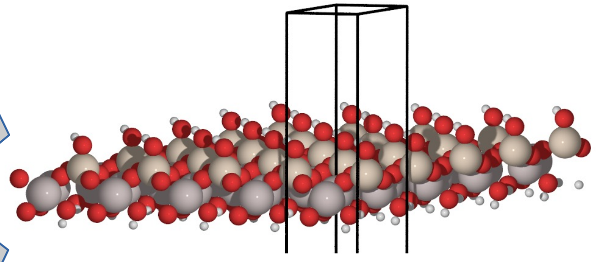

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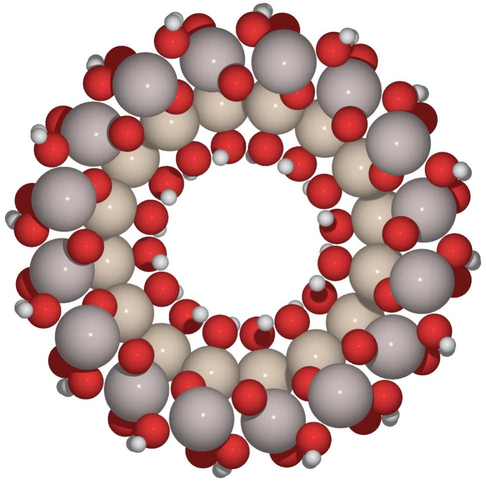

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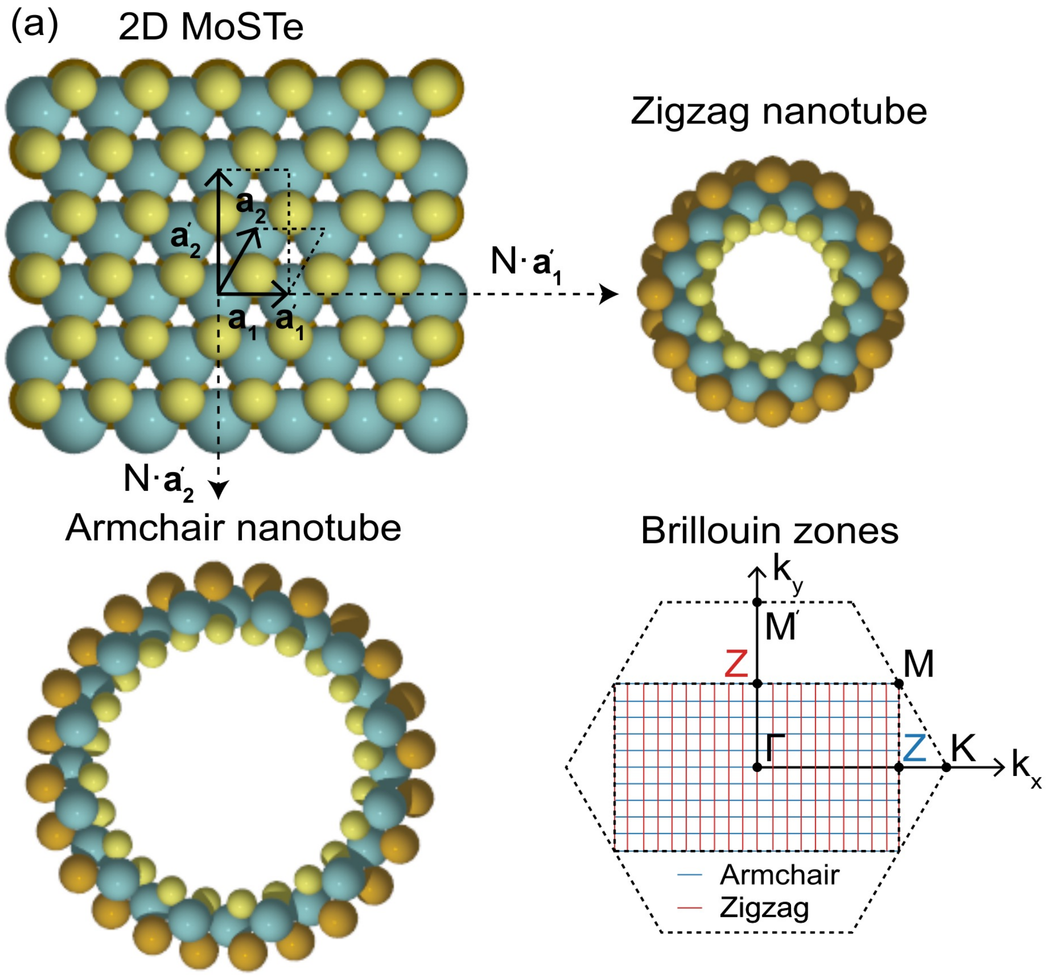
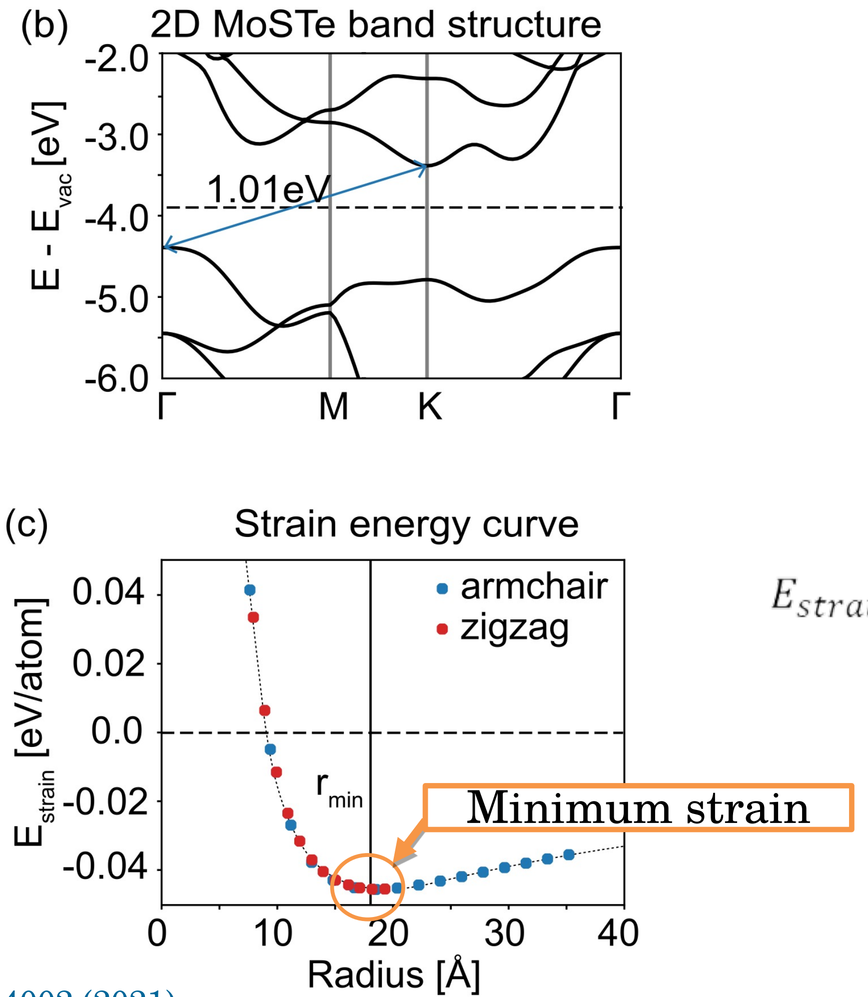
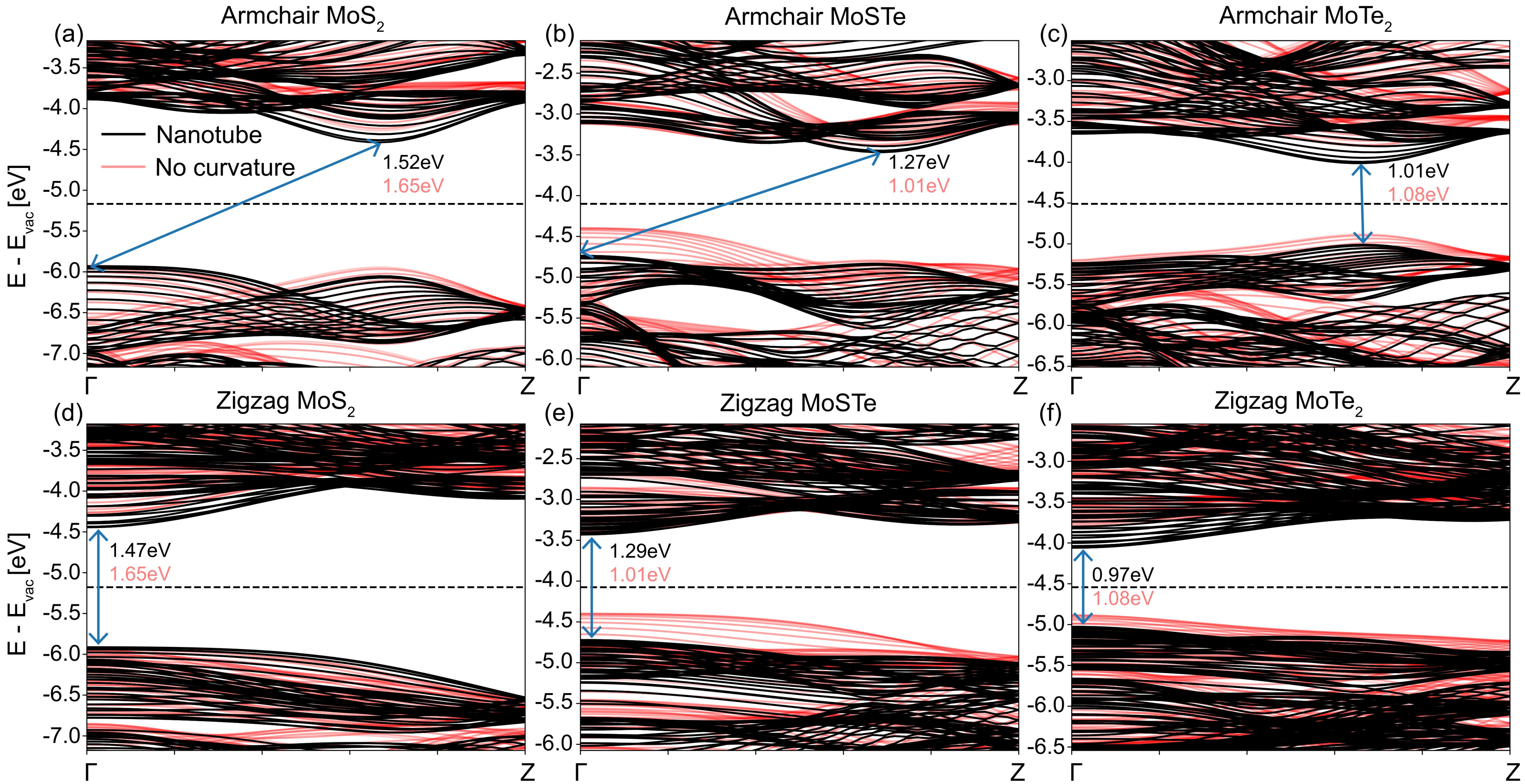




$$E_{strain} = \frac{E_{tube}}{N_{tube}} - \frac{E_{\infty-sheet}}{N_{\infty-sheet}}$$

Mikkelsen, Bölle, Thygesen, Vegge, and Castelli, *Phys. Rev. Mater* **5**, 014002 (2021)

Janus Nanotube VS Parent Sheets



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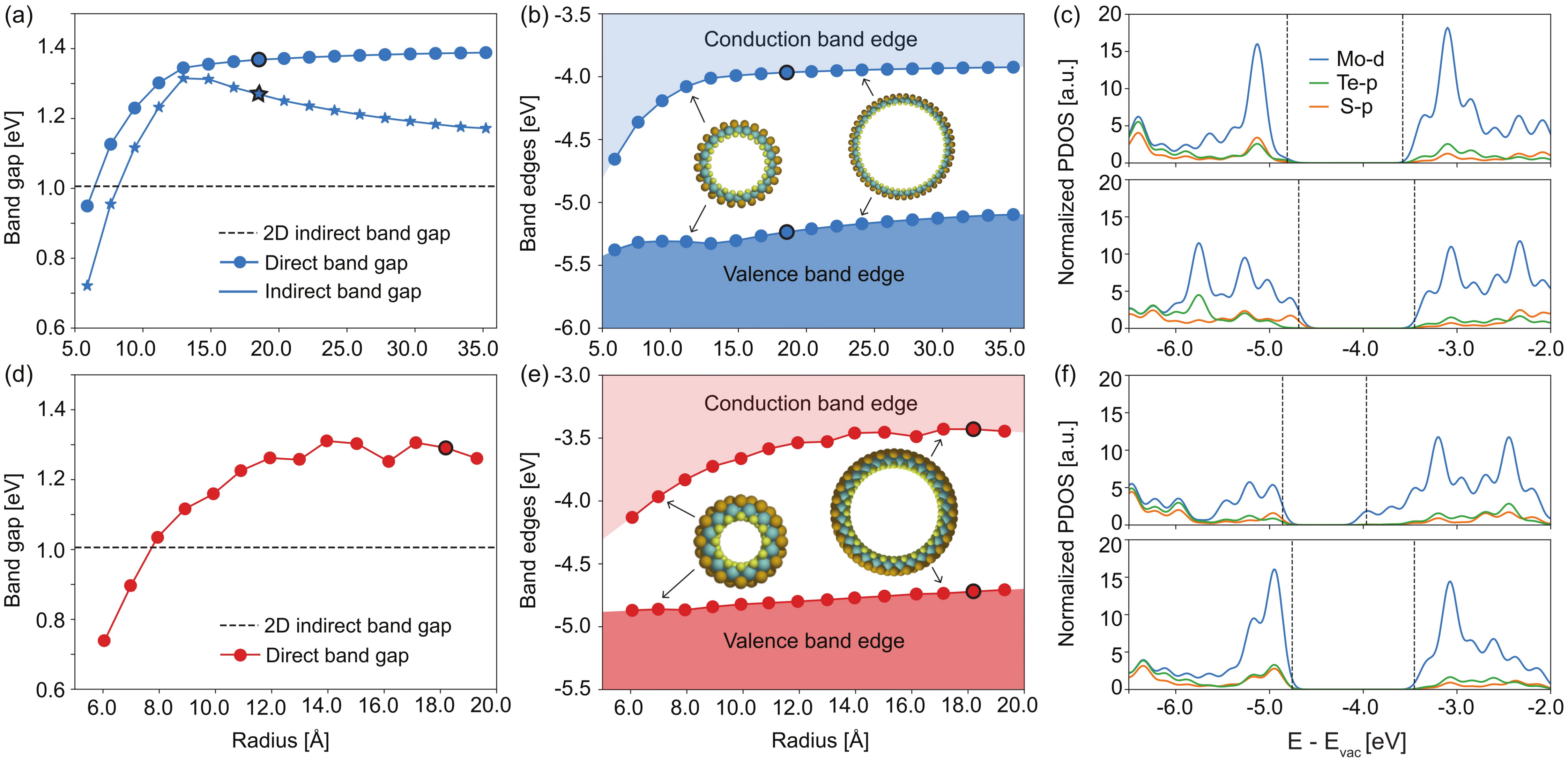

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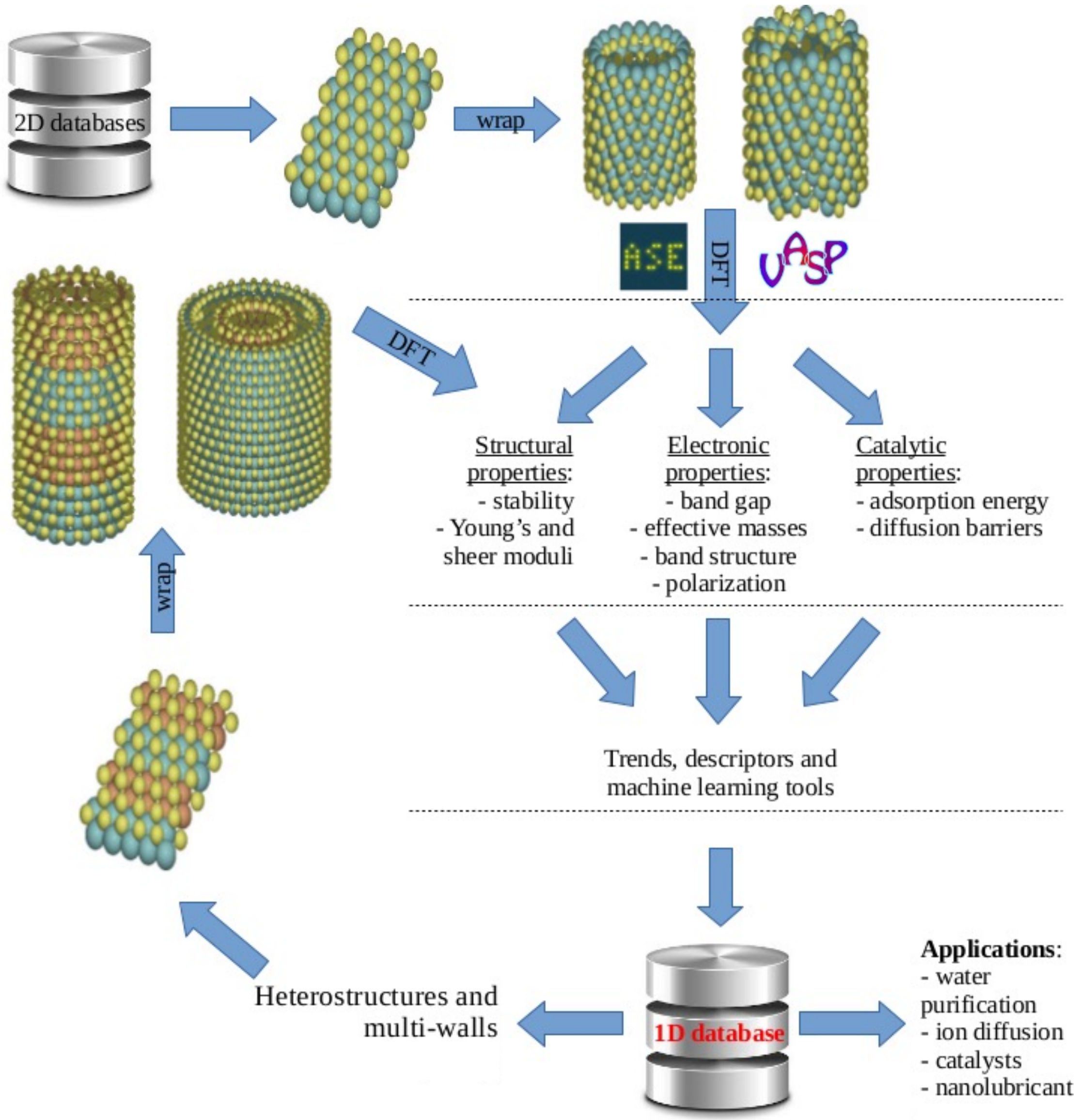
Discovery of Nanometric Nanotubes – The Workflow



Bölle, Mikkelsen, Thygesen, Vegge, and Castelli, *npj Comp. Mater.* **7**, 41 (2021)

Why a workflow?

- manages calculations
- manage dependences
- use always the same parameters
- error handling
- collect and share the data

Myqueue:

http://myqueue.readthedocs.io

Atomic Simulation Environment (ASE):

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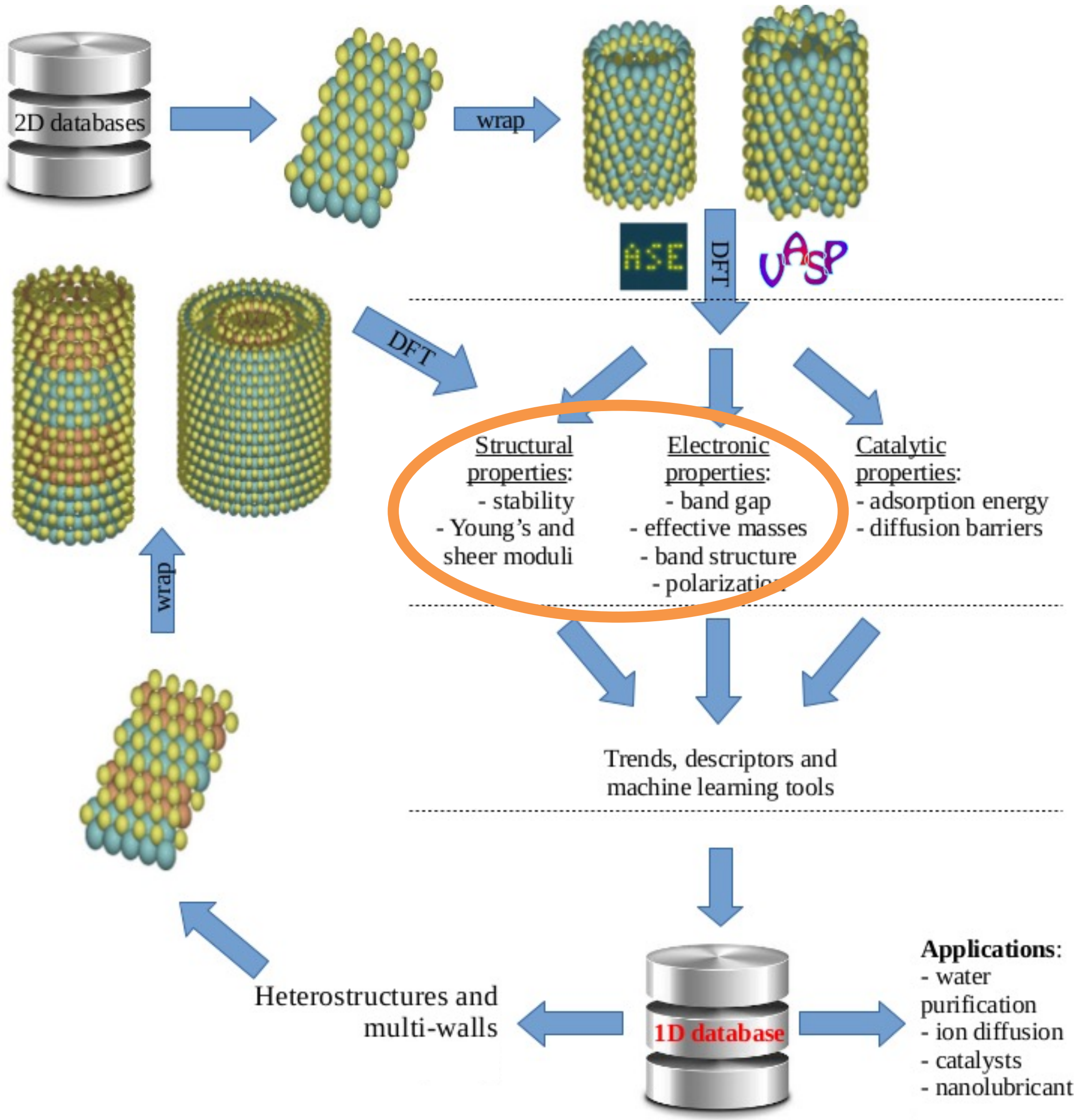

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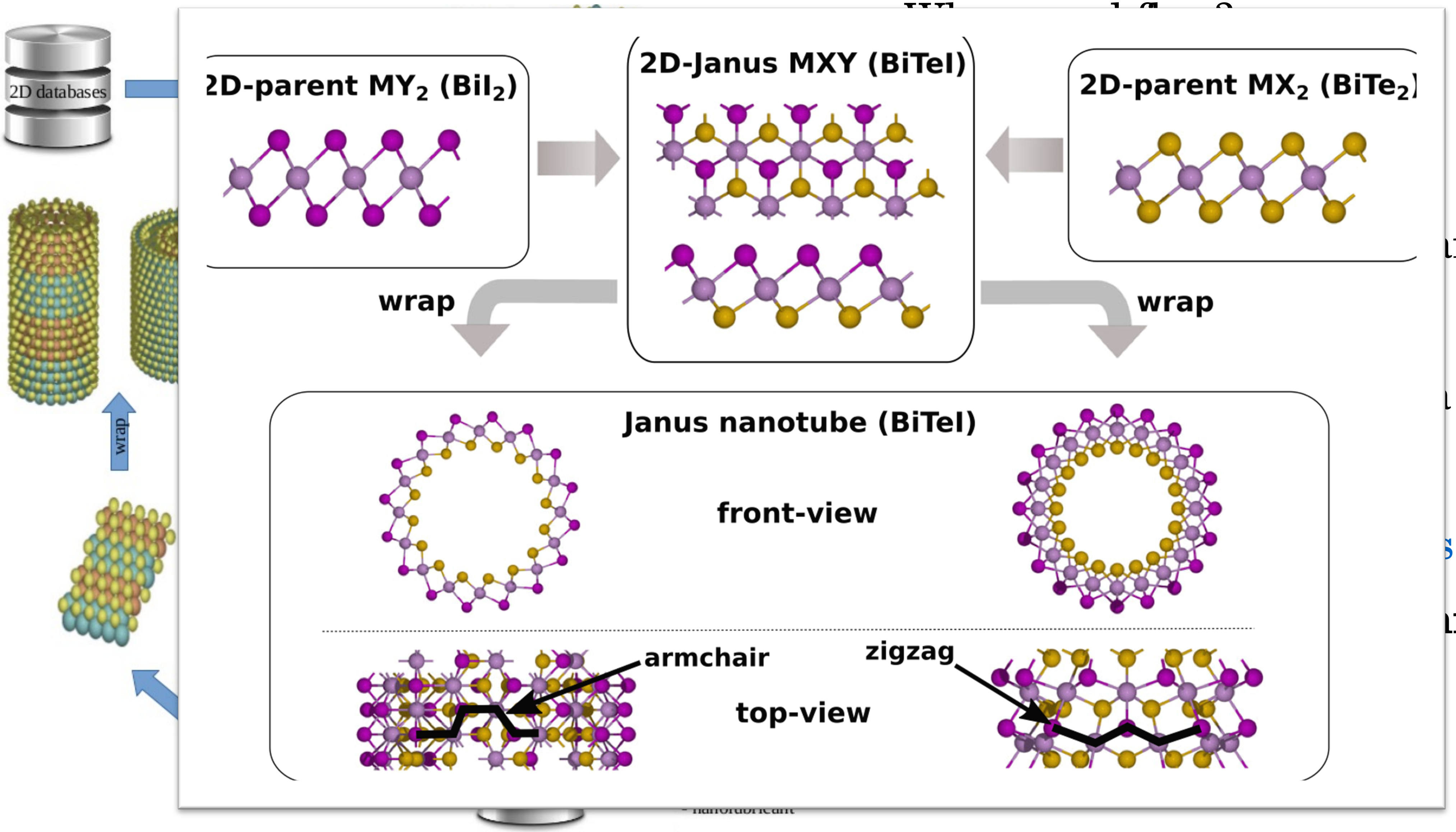

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ment (ASE):

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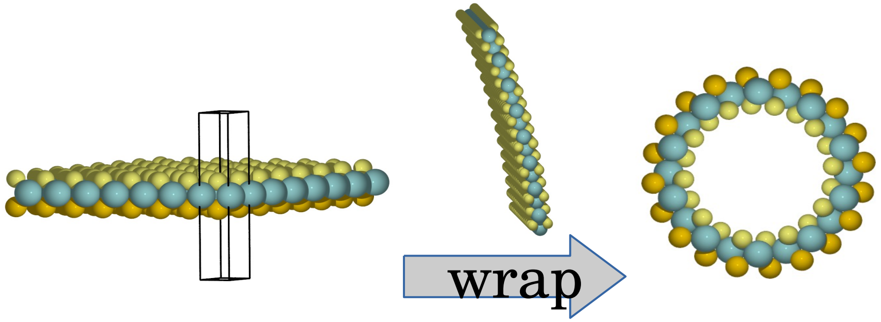
Dichalcogenide Nanotubes



MoSSe

S – Mo – Se

Ternary MXY (X-M-Y) nanotubes:

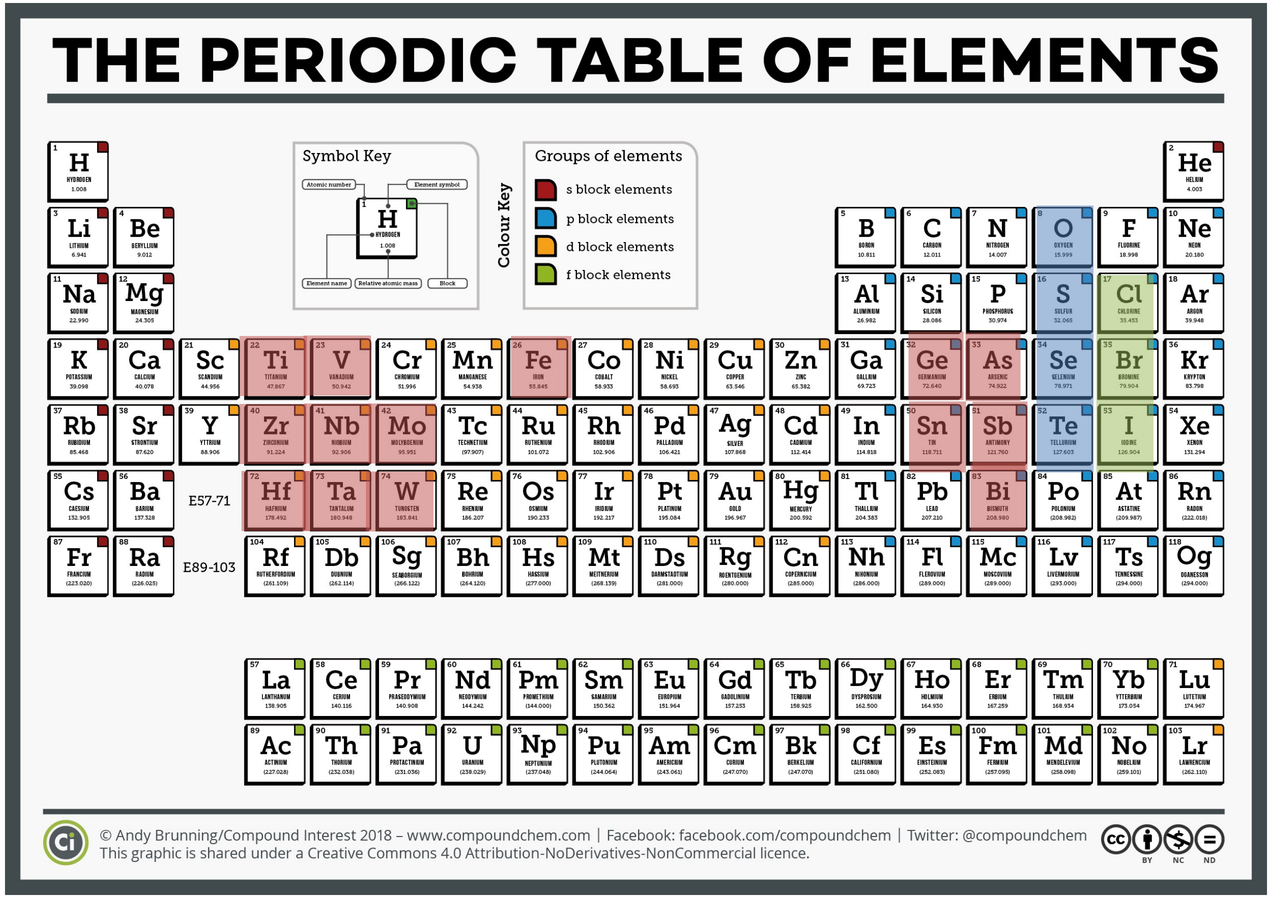
M – 14 metals

XY – Chalcogens (O, S, Se, Te) and Halides (Cl, Br, I)

Two prototype structures: MoS_2 (2H-phase) and CdI_2 (1T-phase)

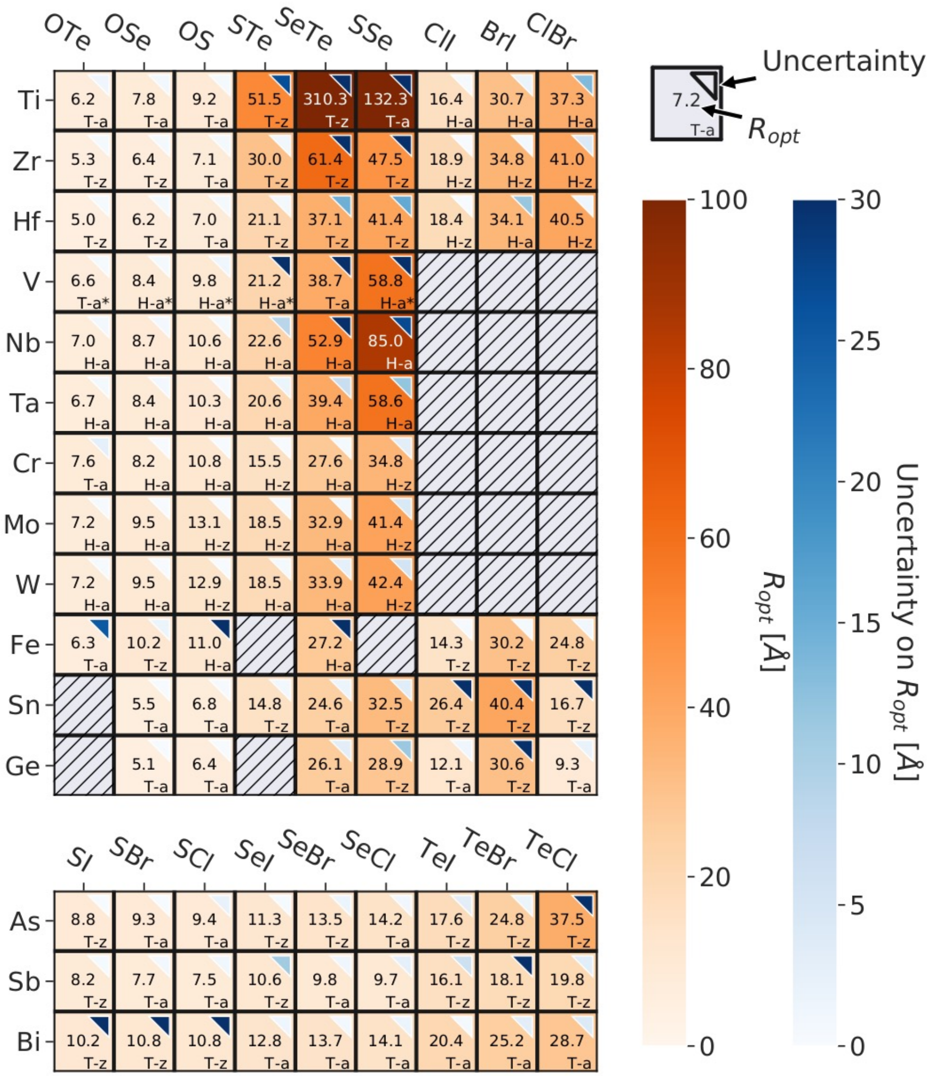
Two wrapping directions: Armchair and Zigzag

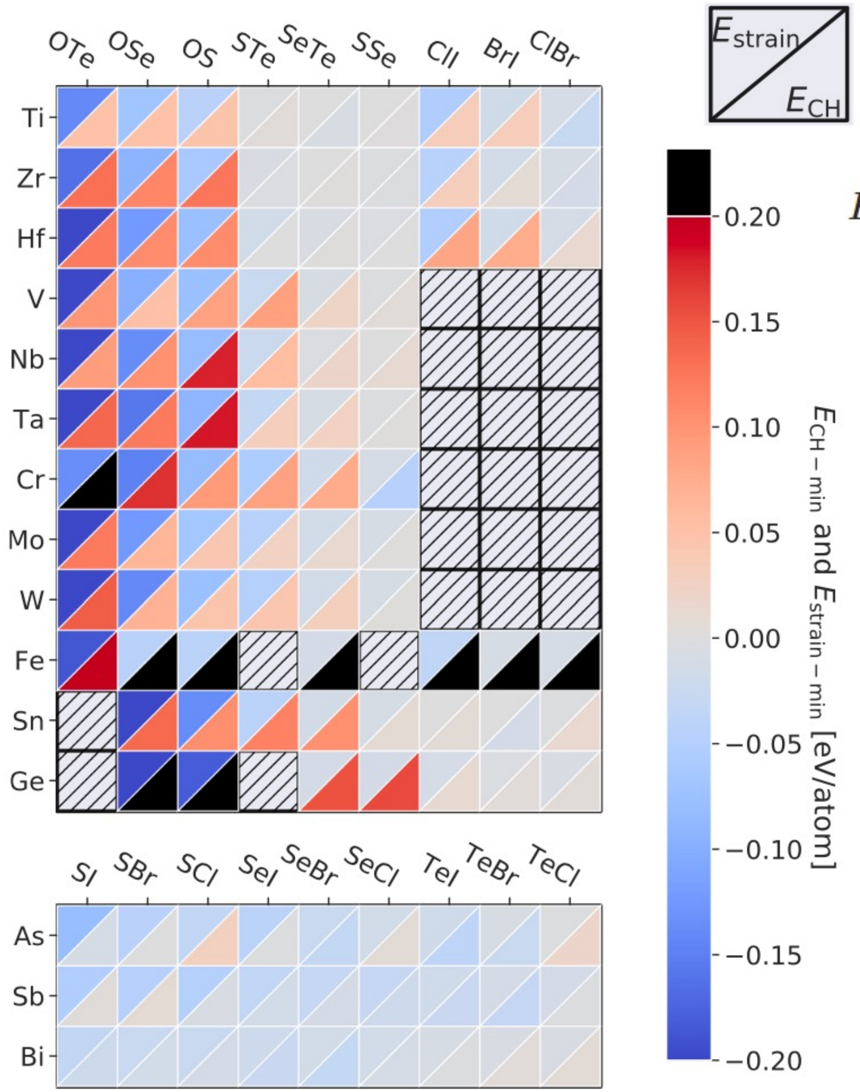
Aim: radii range ~ 5 – 15 Å



Bölle, Mikkelsen, Thygesen, Vegge, and Castelli, *npj Comp. Mater.* **7**, 41 (2021)

Dichalcogenide Nanotubes – Strain and Formation Energies

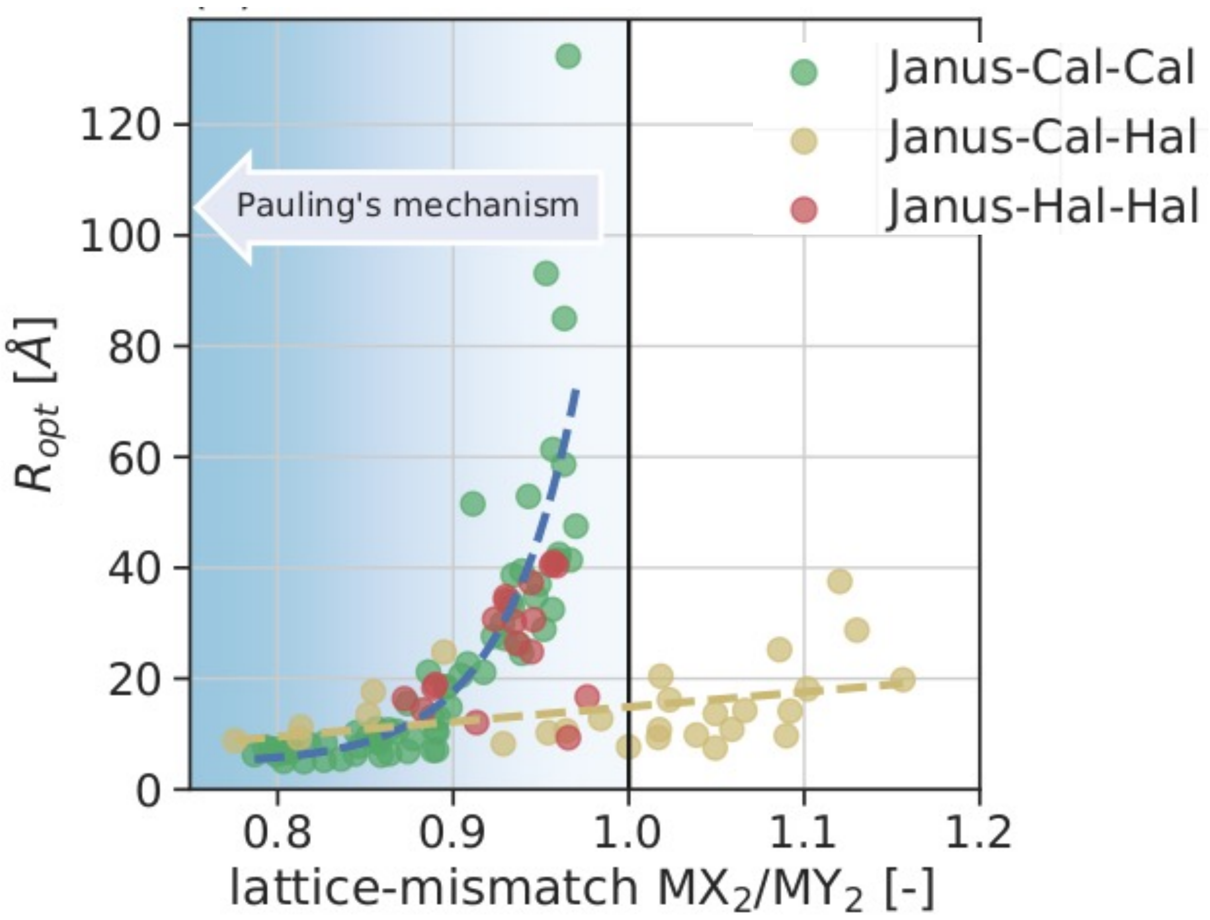




$$E_{\text{strain}}(R) = \frac{a}{R^2} + \frac{b}{R},$$

Bölle, Mikkelsen, Thygesen, Vegge, and Castelli, *npj Comp. Mater.* **7**, 41 (2021)

Dichalcogenide Nanotubes – Formation Mechanism



Trends:

OTe < OSe < OS < STe < SeTe < SSe

???

ClI < BrI < ClBr

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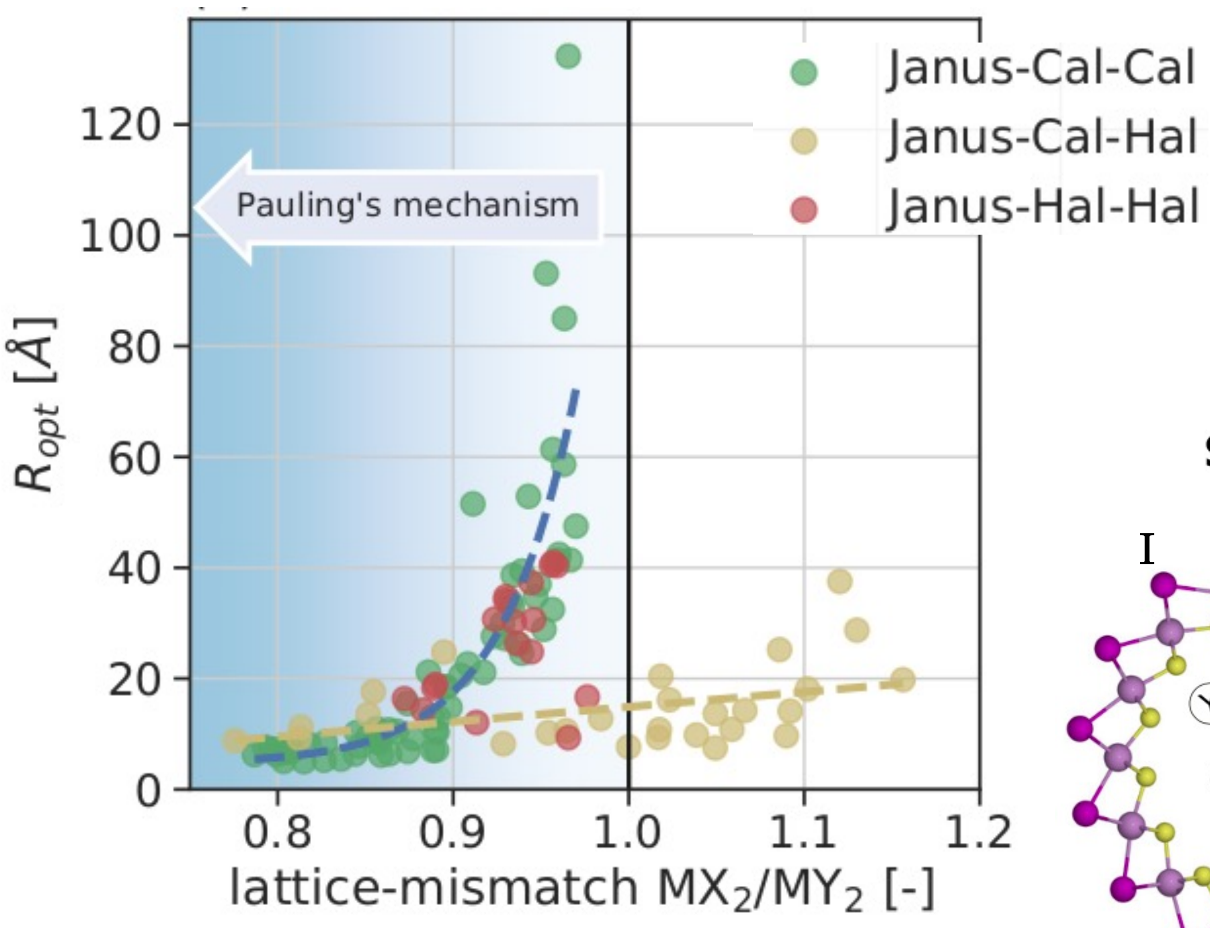

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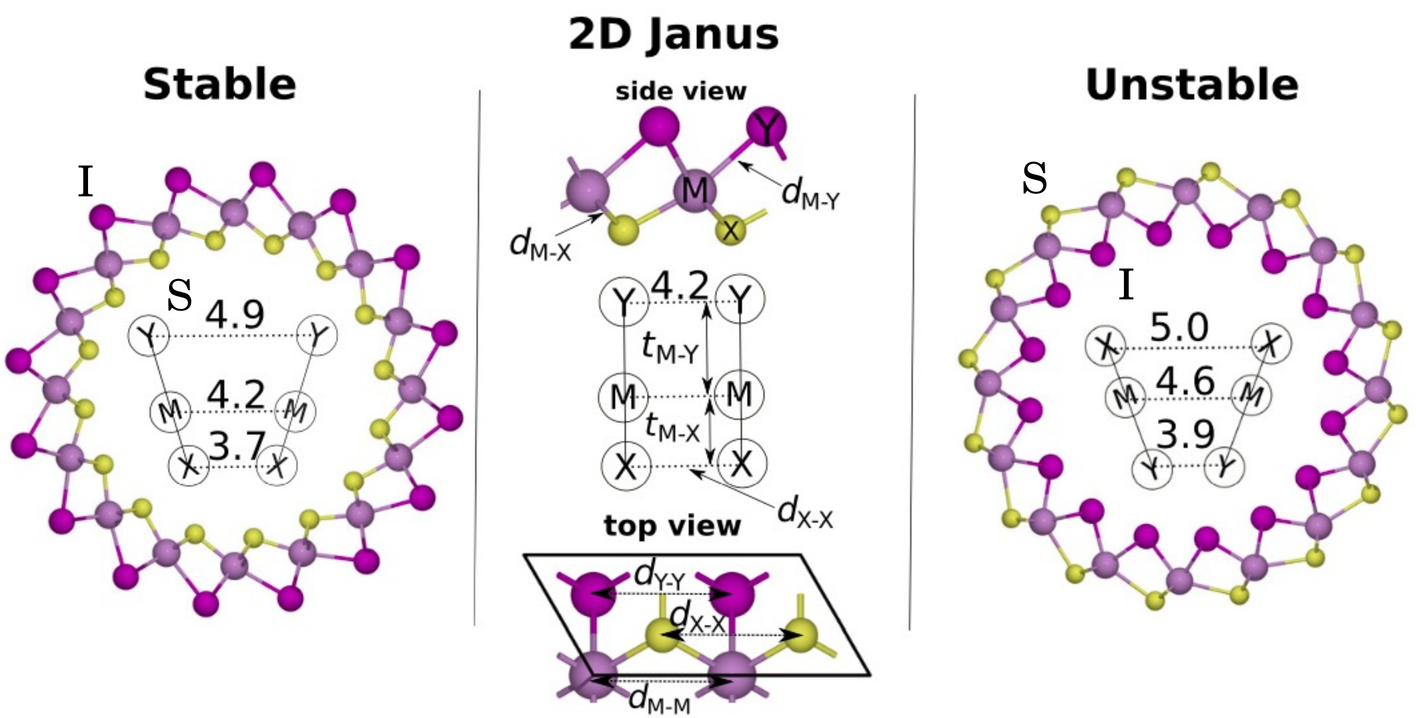

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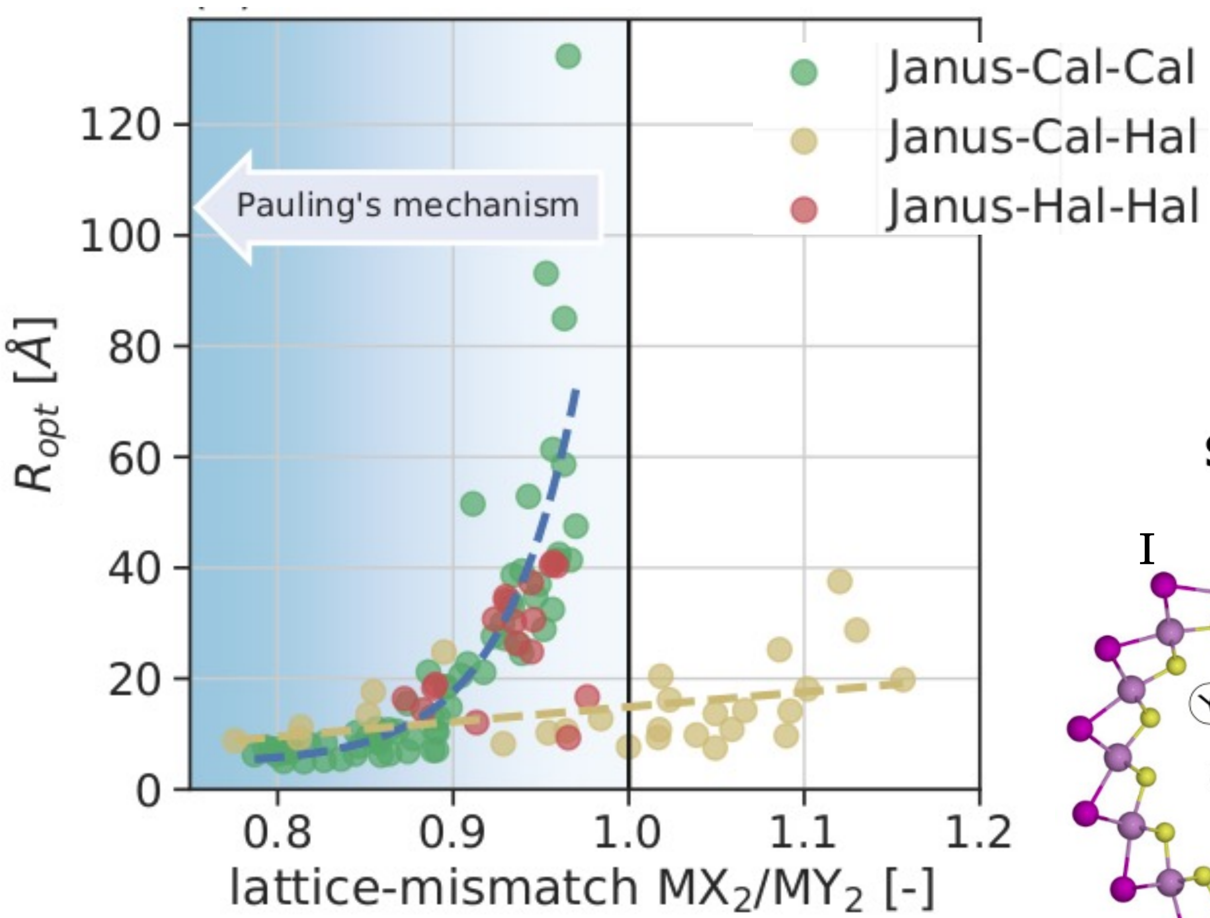

Trends:

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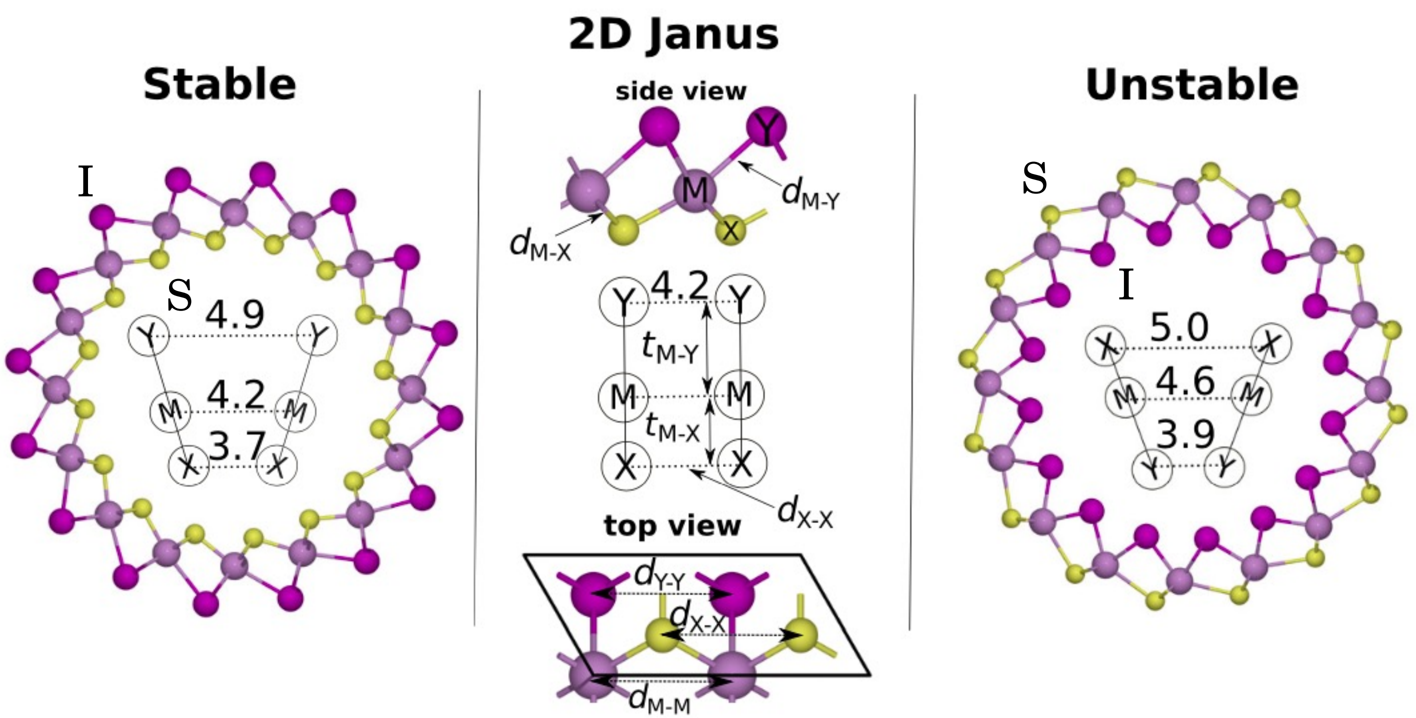
Element with stronger bonds determines wrapping direction

ClI < BrI < ClBr

BiSI



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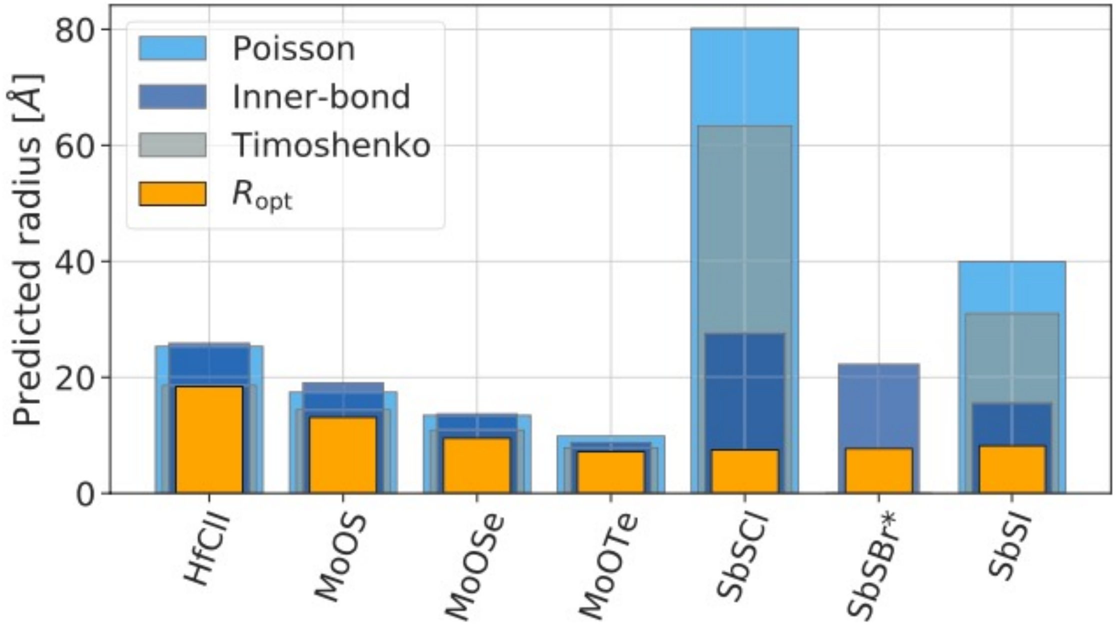
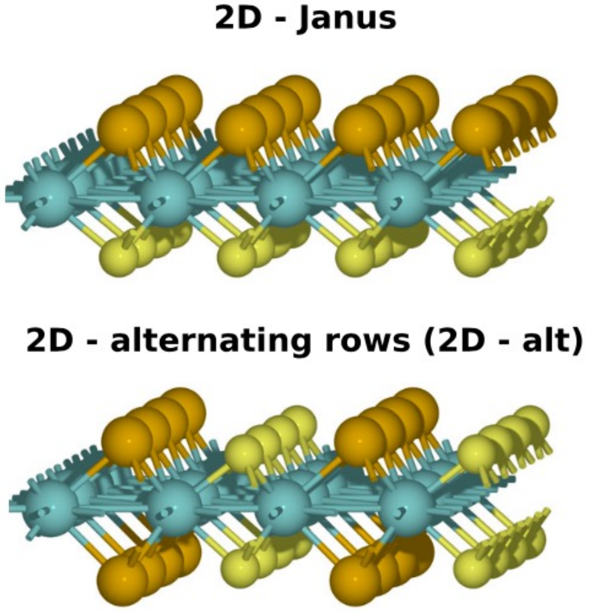
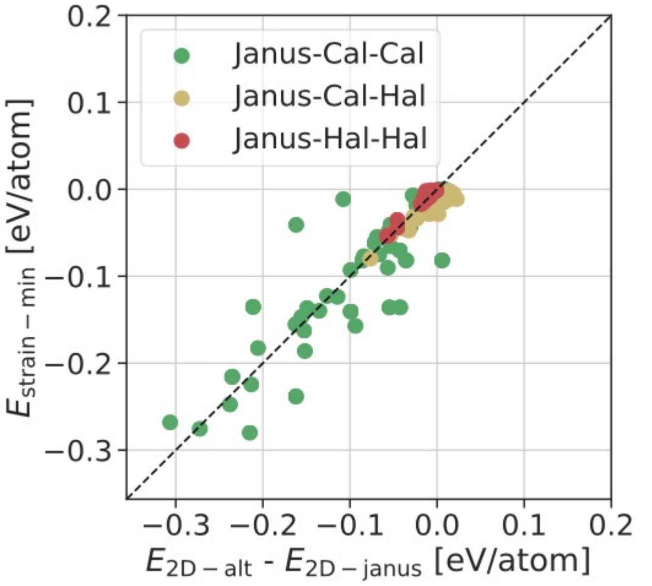
Dichalcogenide Nanotubes – Prediction of Radii and Energies



Timoshenko: lattice mismatch between MX_2 and MY_2 2D sheets

Inner-bond: lattice mismatch between MXY and MY_2 2D sheets





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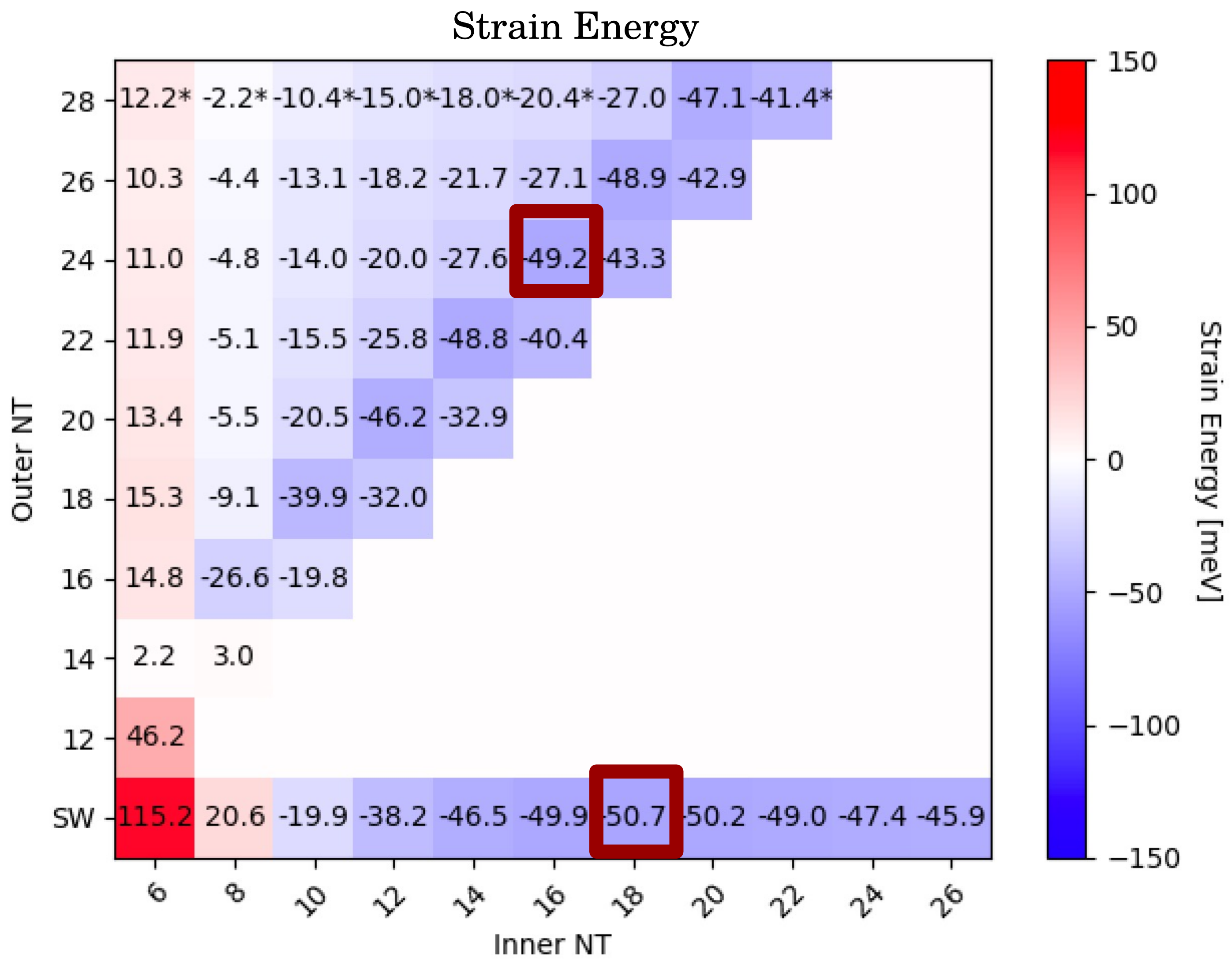
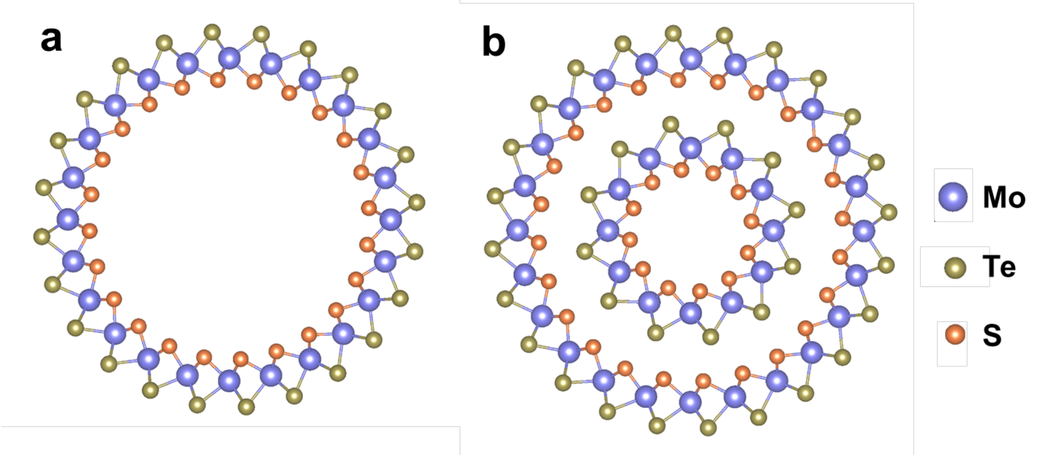
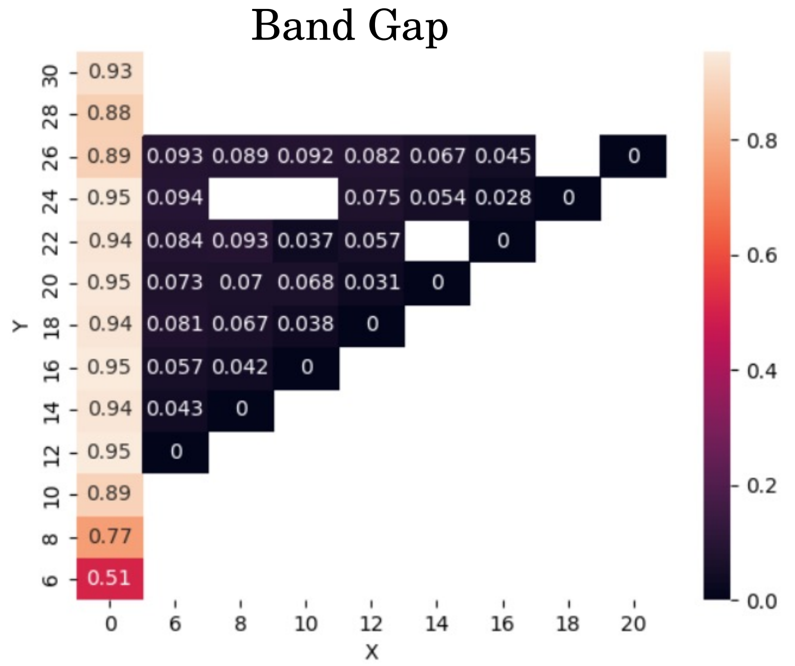
Multiwalls Nanotubes: MoSTe





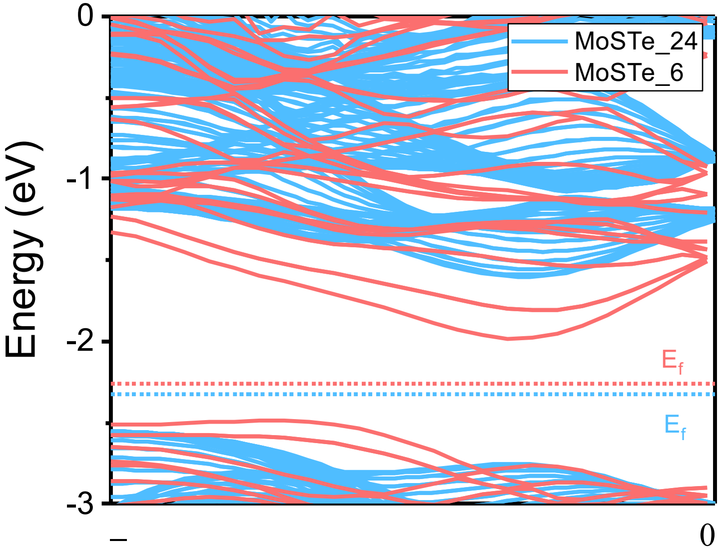


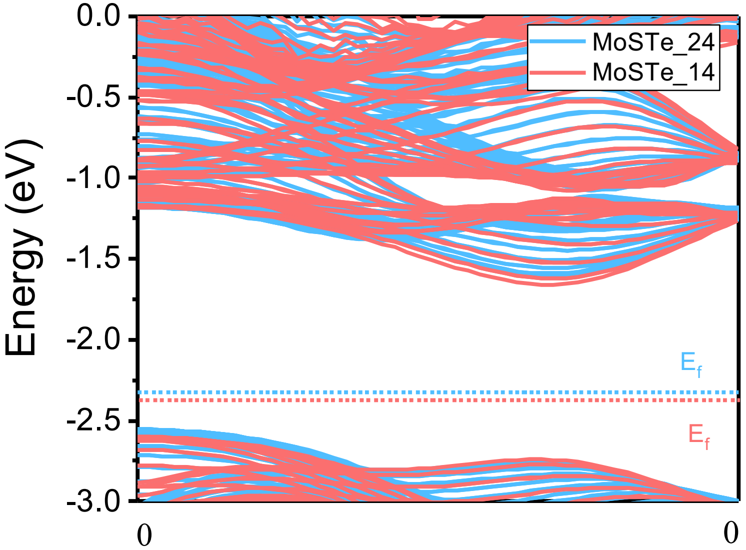
Lan, Kapunan, Bölle, and Castelli, in preparation (2022)

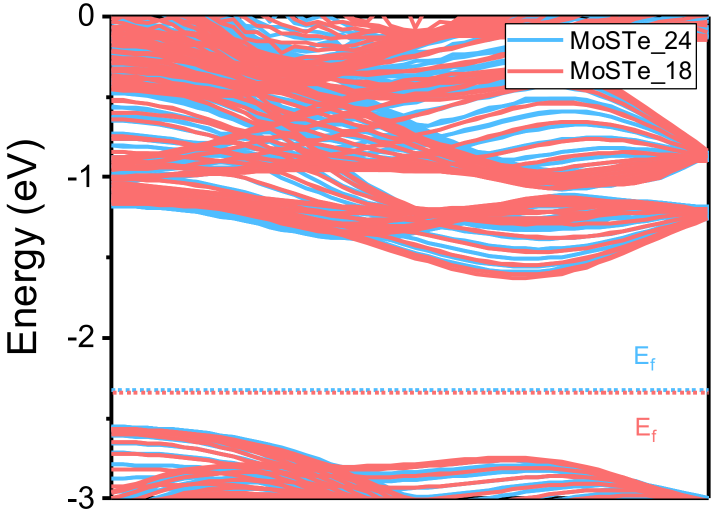
Multiwalls Nanotubes: MoSTe – Band Gap

What is happening?

Single wall nanotube







Biwall nanotube

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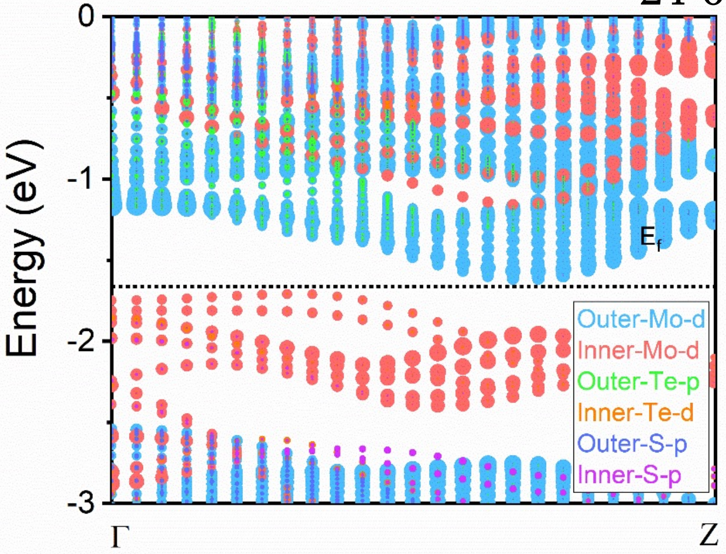
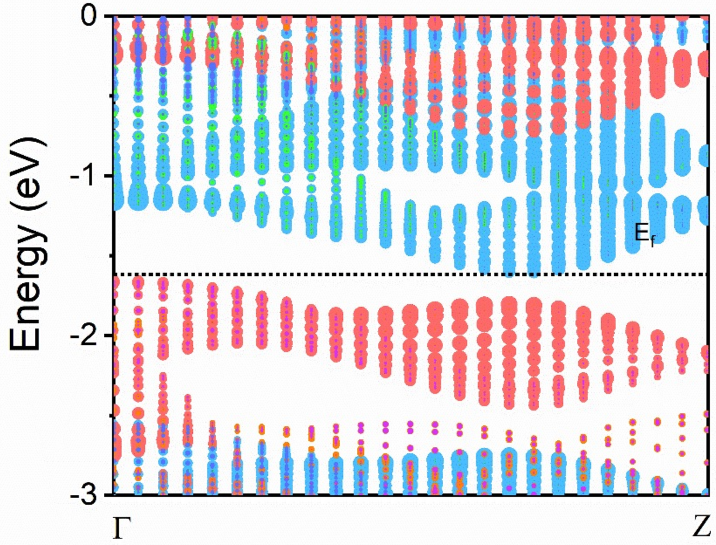


24-14



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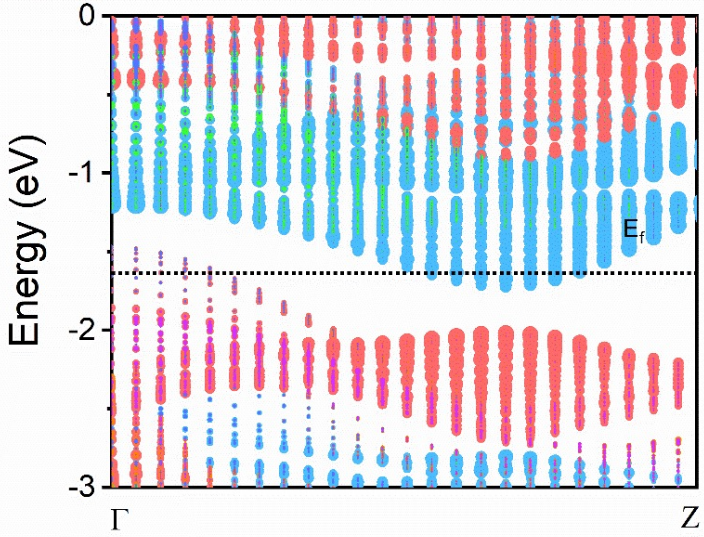
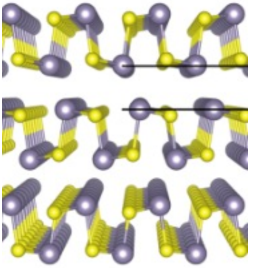
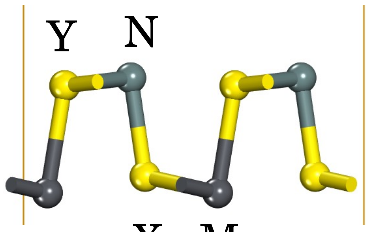


Beyond the MoS_2/CdI_2 Nanotubes – IV-VI Janus Tubes



Exfoliate

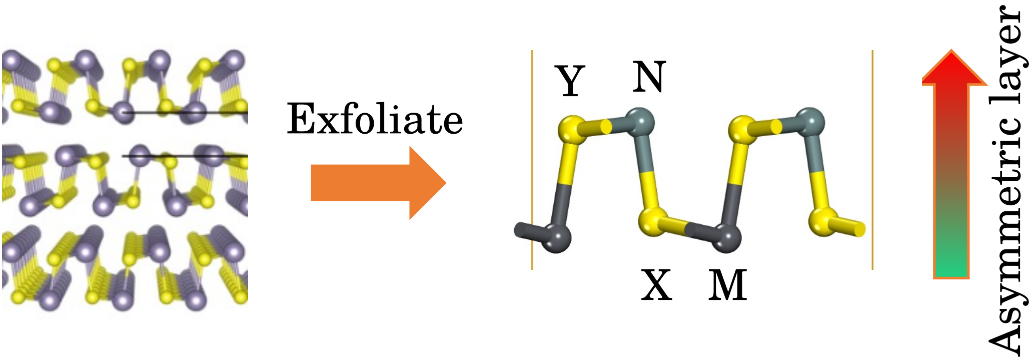


3D - Bulk

2D

Zheng, Bölle, Vegge, and Castelli, in preparation (2022)

Beyond the MoS_2/CdI_2 Nanotubes – IV-VI Janus Tubes



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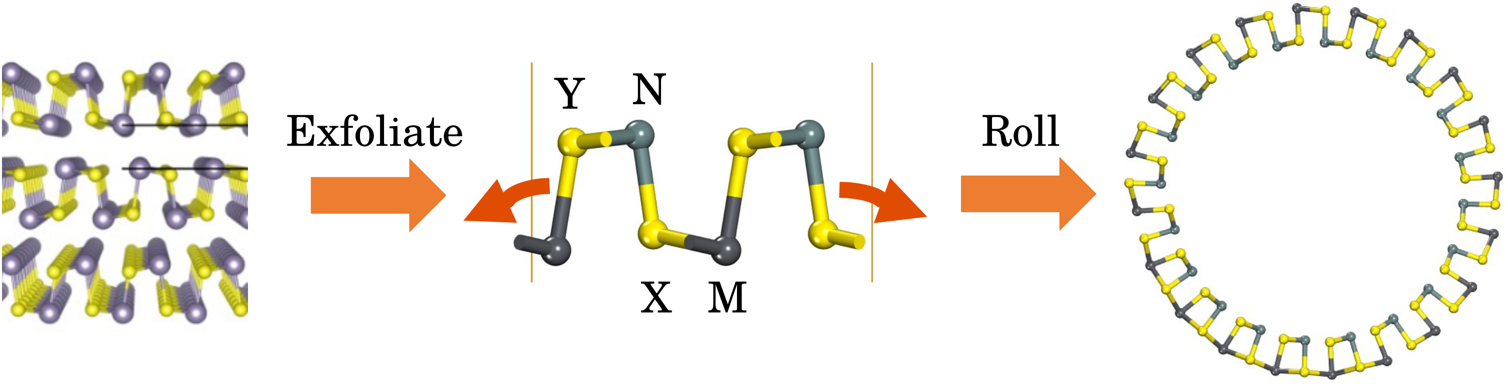
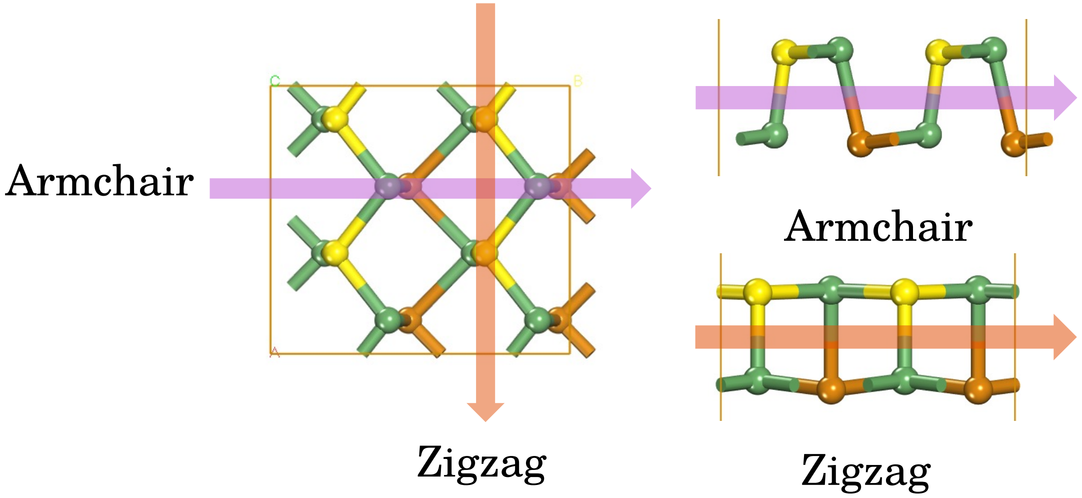
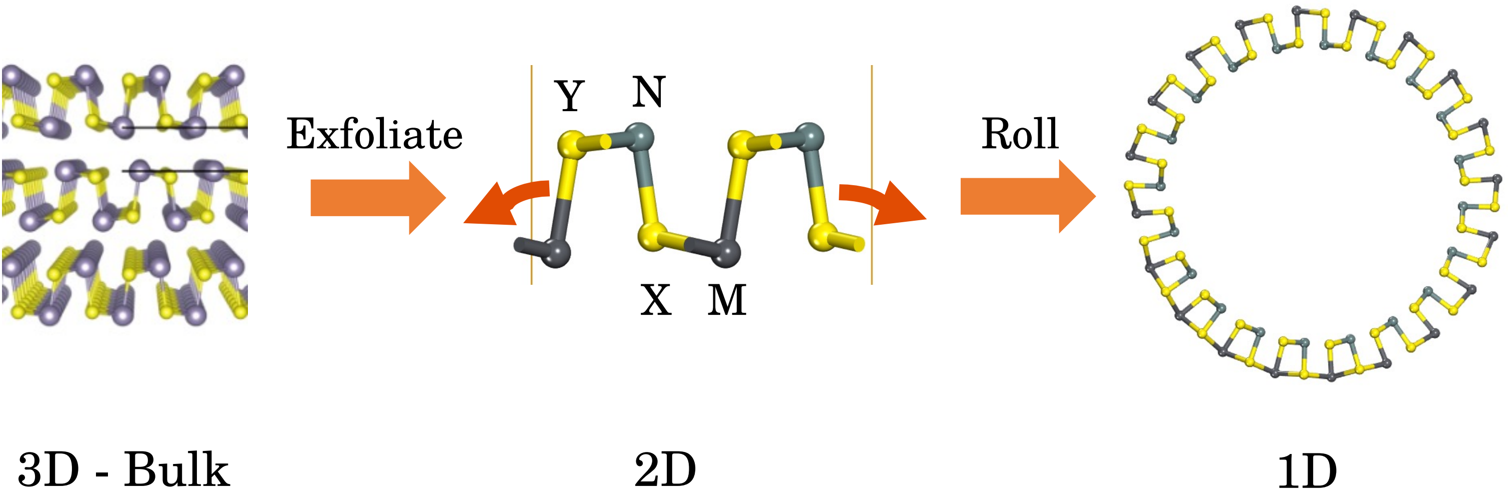


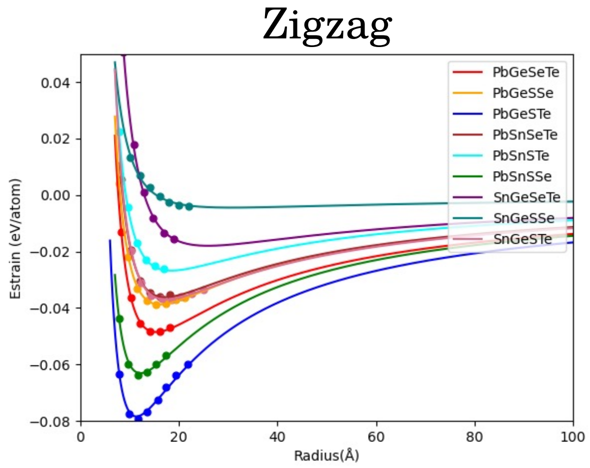
3D - Bulk　　2D　　1D

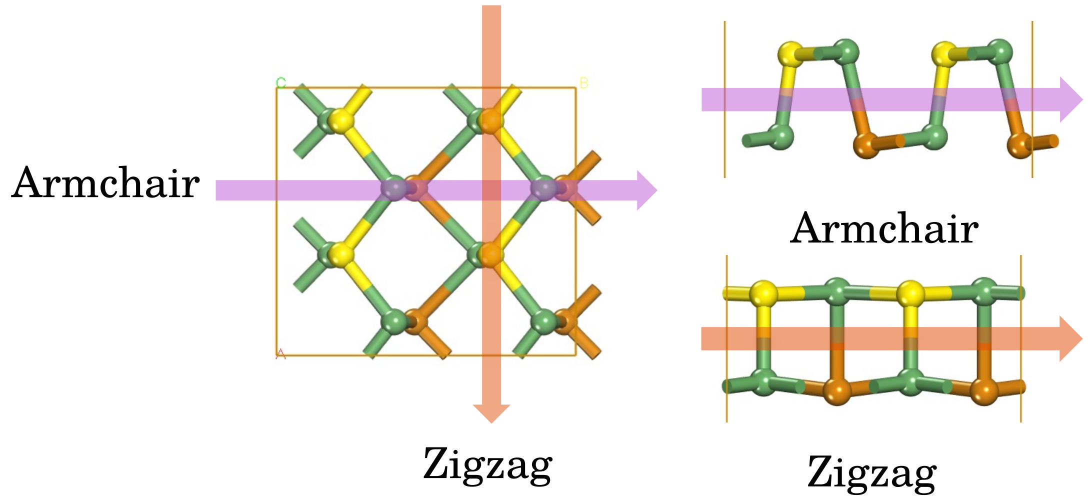


Zheng, Bölle, Vegge, and Castelli, in preparation (2022)

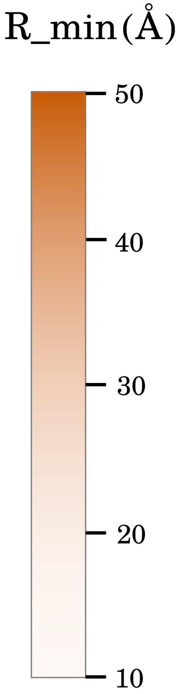
Beyond the MoS_2/CdI_2 Nanotubes – IV-VI Janus Tubes





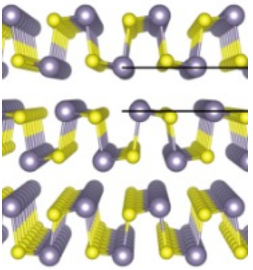


	SeTe	SSe	STe	S_2	Se_2	Te_2
PbGe	15.37	16.17	11.34	23.77	25.15	25.31
PbSn	25.91	30.76	17.3	67.69	464.28	110.92
SnGe	17.16	18.42	12.19	30.75	32.4	32.38
Pb_2	23.09	41.74	18.62			
Sn_2	24.16	41.6	18.6			
Ge_2	22.12	30.98	17.32			

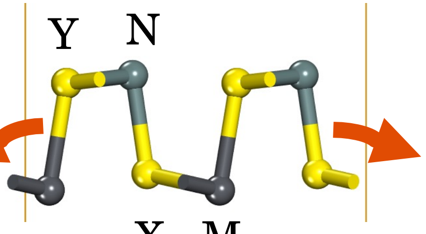


Zheng, Bölle, Vegge, and Castelli, in preparation (2022)

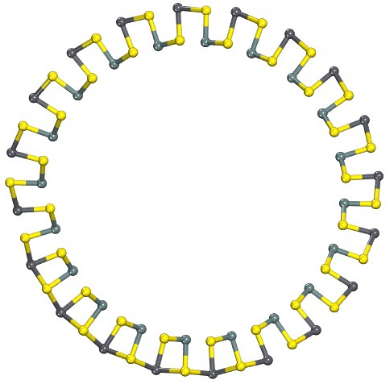
Beyond the MoS_2/CdI_2 Nanotubes – IV-VI Janus Tubes



Exfoliate



Roll

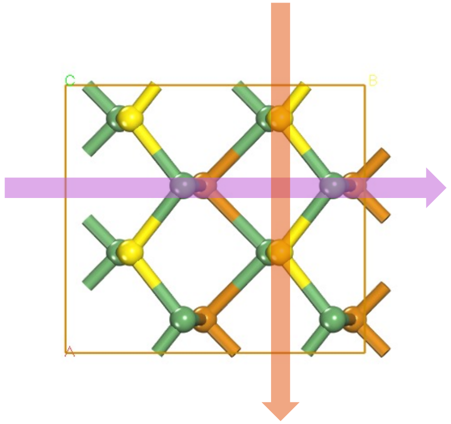


3D - Bulk

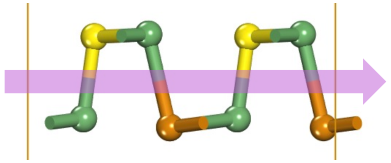
2D

1D

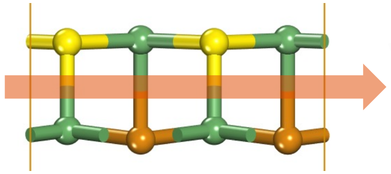
Armchair



Zigzag



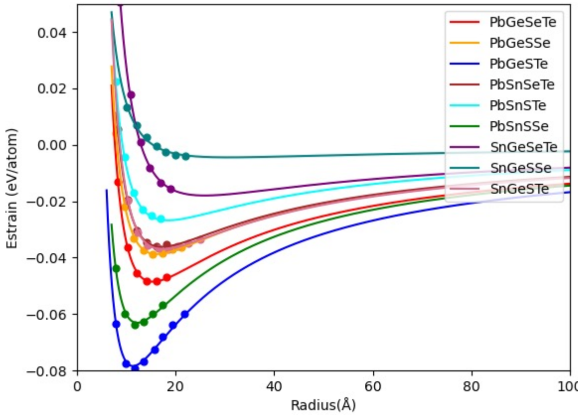
Armchair



Zigzag

What is the formation mechanism?

Zigzag



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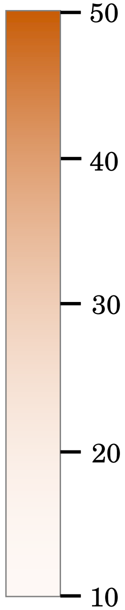
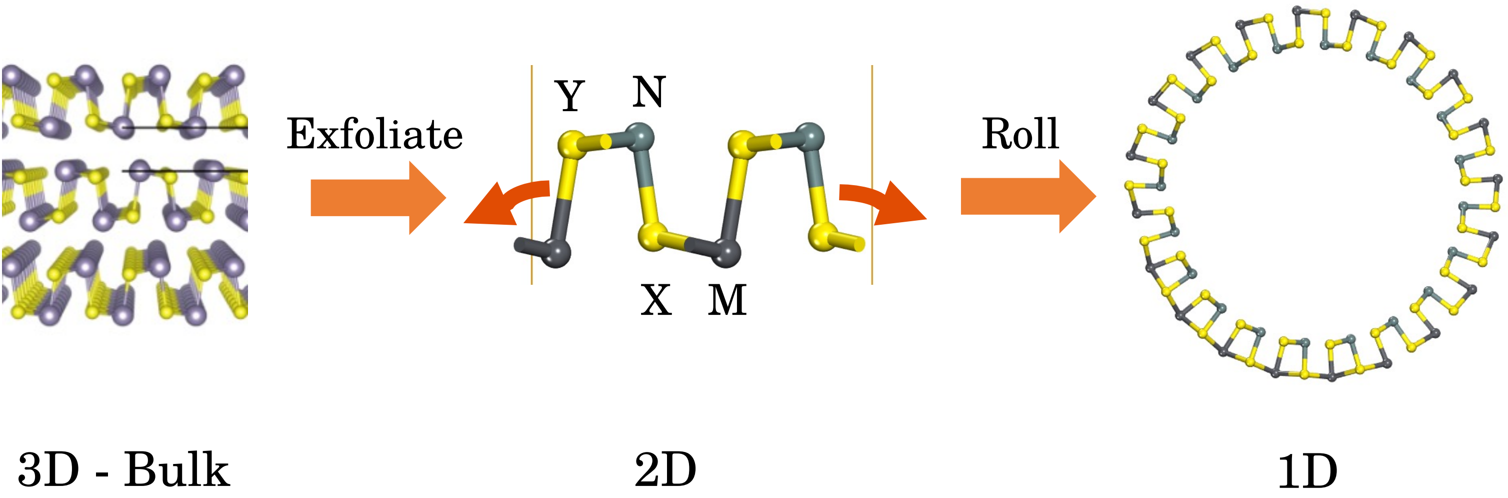
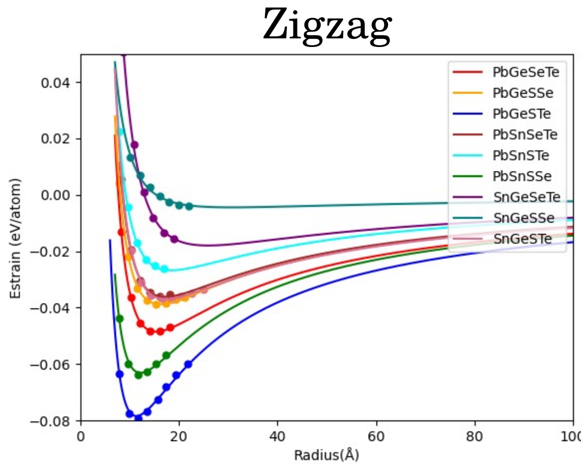
R_min(Å)

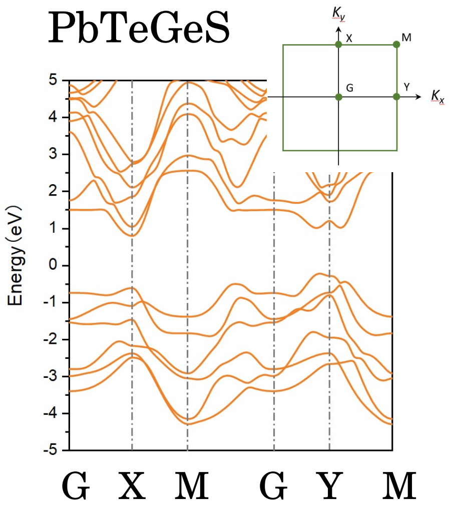


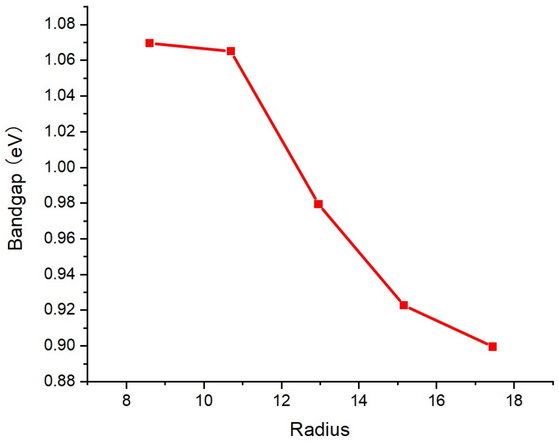
Zheng, Bölle, Vegge, and Castelli, in preparation (2022)

Beyond the MoS_2/CdI_2 Nanotubes – IV-VI Janus Tubes









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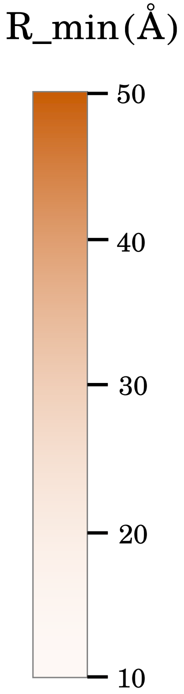
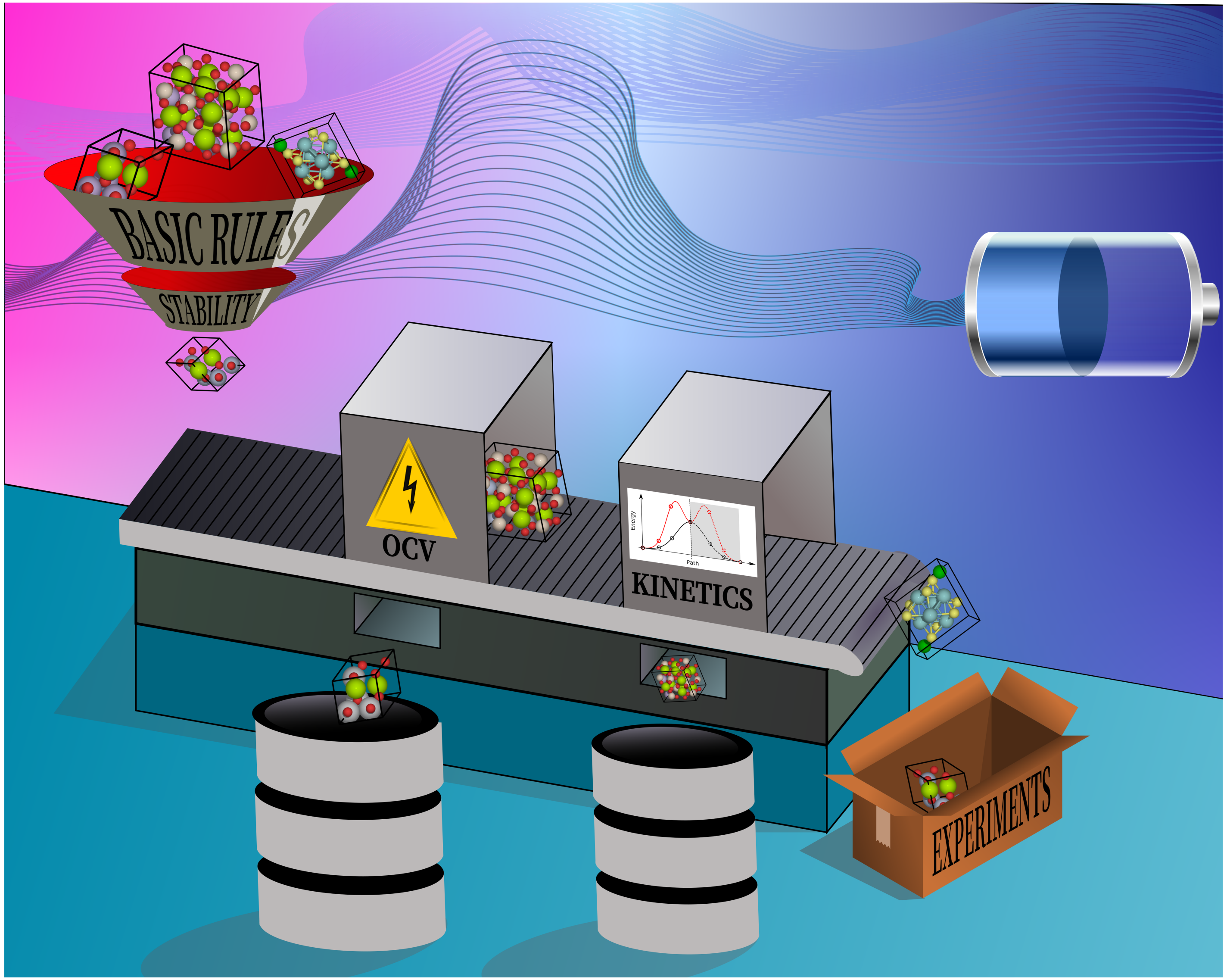


Zheng, Bölle, Vegge, and Castelli, in preparation (2022)

Autonomous Discovery of Battery Electrodes



Bölle, Mathiesen, Nielsen, Vegge, Garcia Lastra, and Castelli, *BatteriesSupercaps* ***3***, *488* (2021)

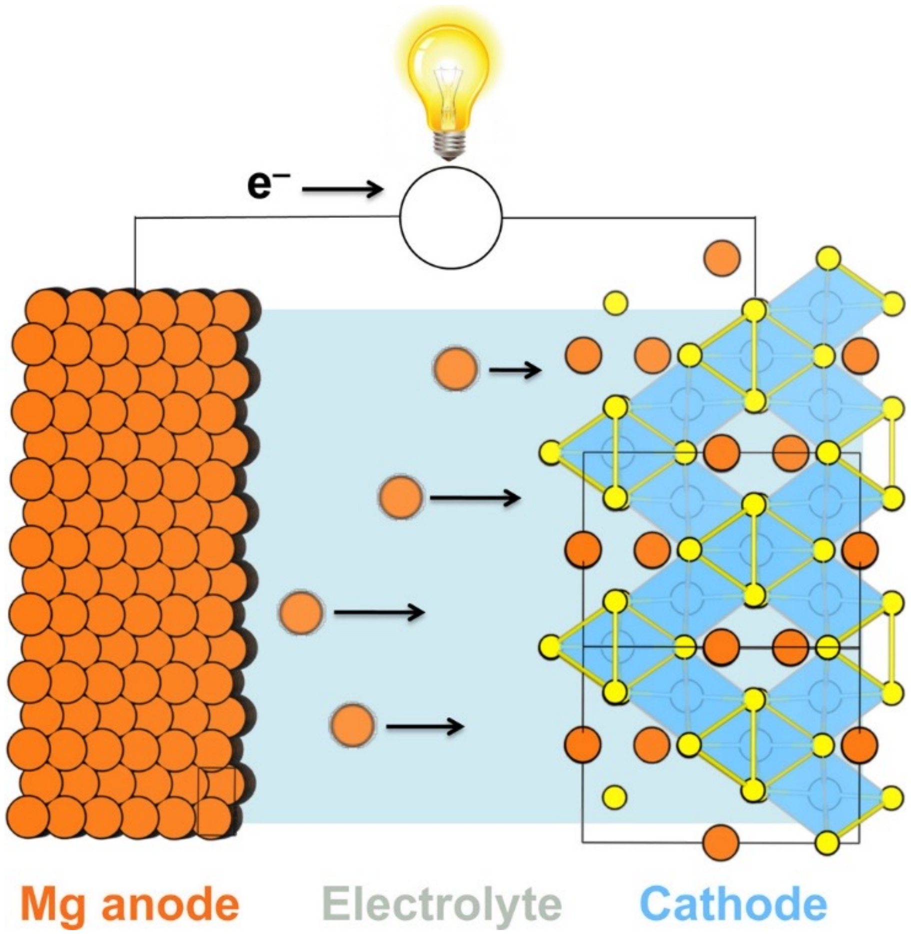
Cathode Materials for Mg-ion Batteries

Why Mg-ion Batteries?

- Multivalent battery
- Increased capacity compared to LIB
- Abundant resources

Main challenges?

- Unstable electrolytes
- Poor cathode materials:
  - low open circuit voltage (OCV)
  - low charge/discharge rate



State-of-the-art cathodes:

$Mg_xMo_6O_8$ (0<x<2, Chevrel) – OCV ~ 1.1 V

Canepa *et al.*, *Chem. Rev.* **117**, 4287 (2017)

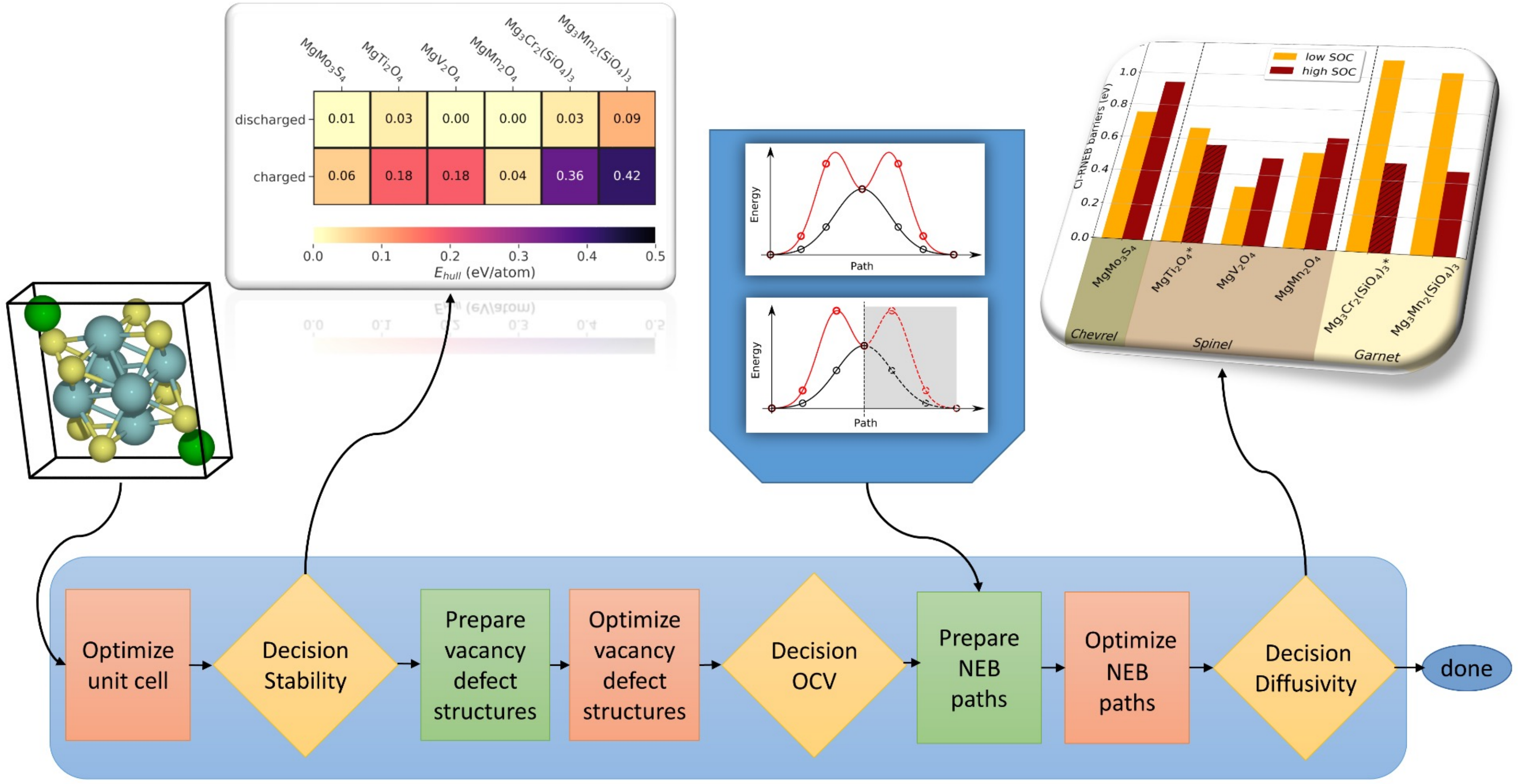
Aurbach *et al.*, *Nature* **407**, 724 (2000)

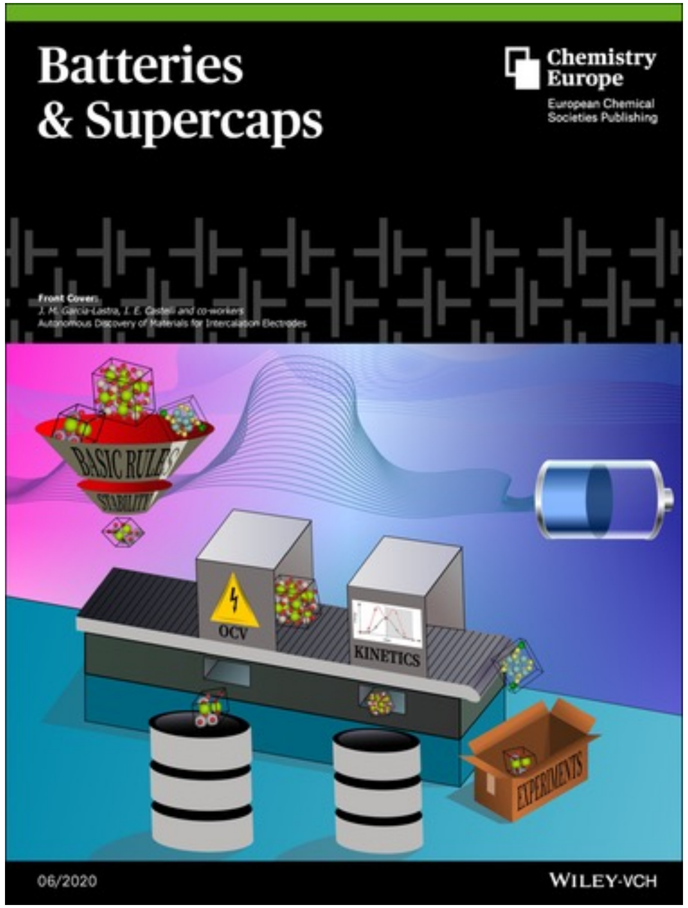
The Workflow

More details: Bölle – Wed 17th, 11.50

Automate the calculations of key thermodynamics and kinetic properties

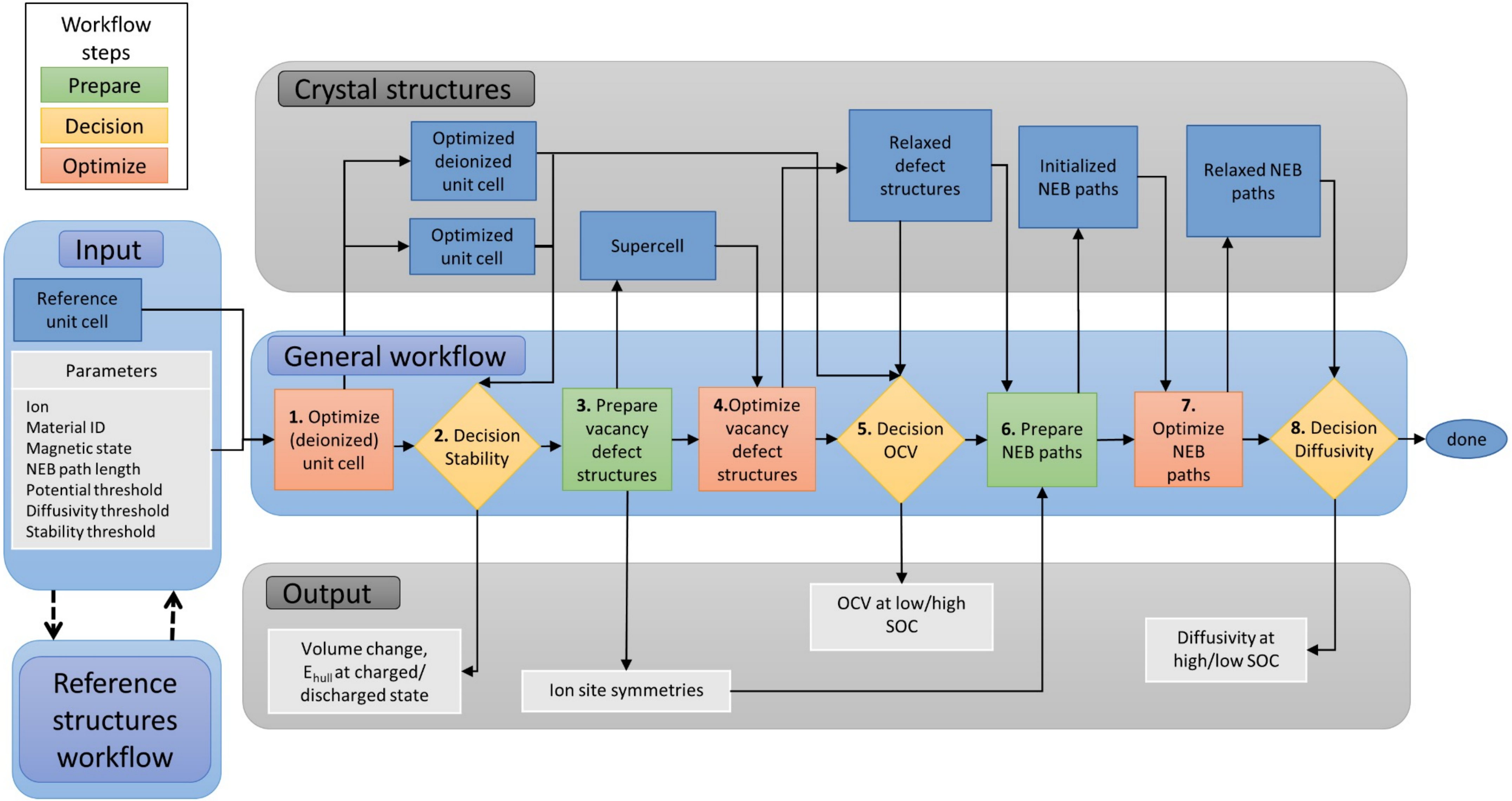
Accelerated screening of known (ICSD/Materials project) or unknown materials (structure prototype)





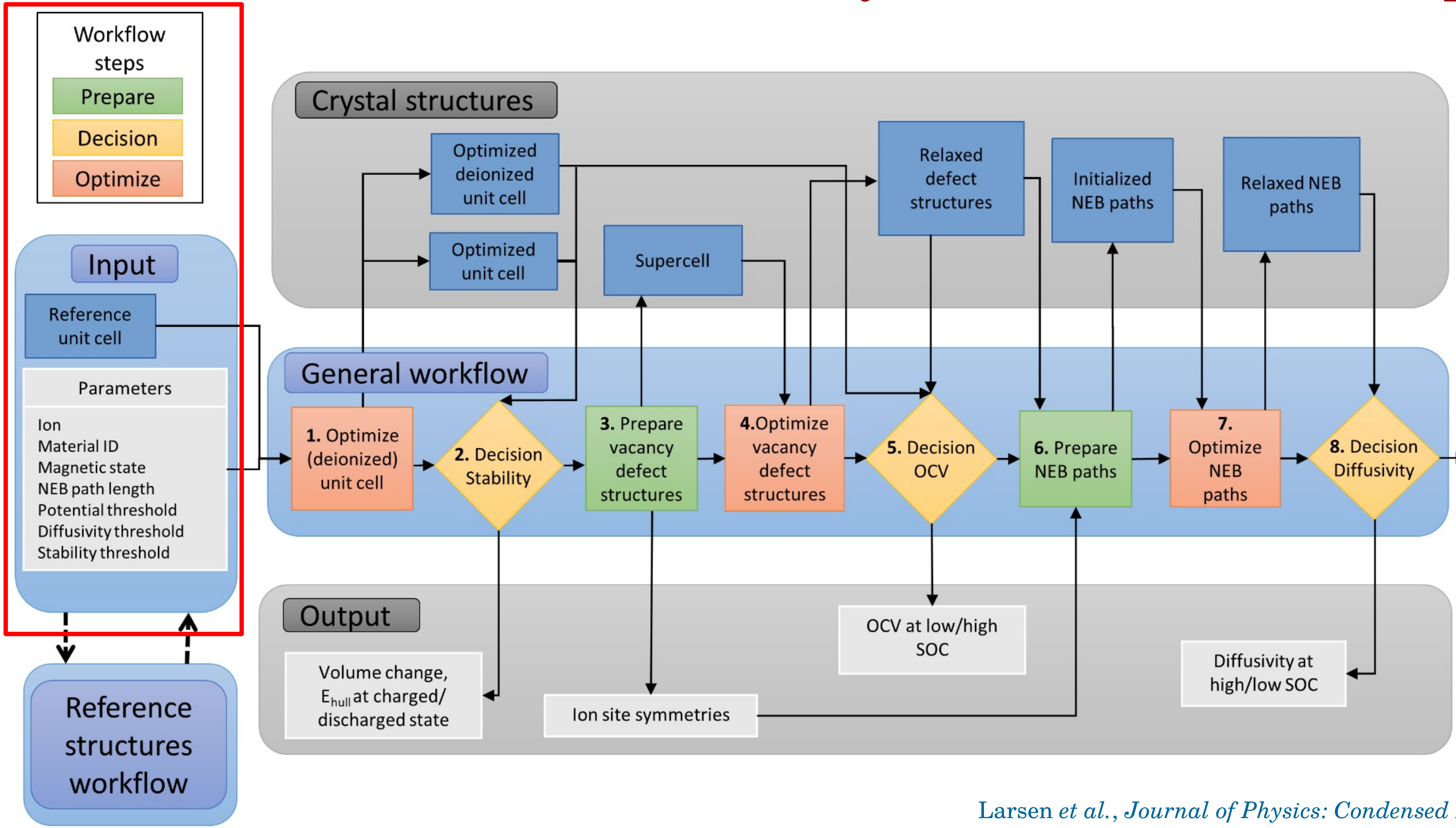
Bölle, Mathiesen, Nielsen, Vegge, Garcia Lastra, and Castelli, *BatteriesSupercaps* ***3**, 488* (2021)

Autonomous Workflow for Thermodynamic and Kinetic Properties



Bölle, Mathiesen, Nielsen, Vegge, Garcia Lastra, and Castelli, *BatteriesSupercaps* ***3**, 488* (2021)

Autonomous Workflow for Thermodynamic and Kinetic Properties

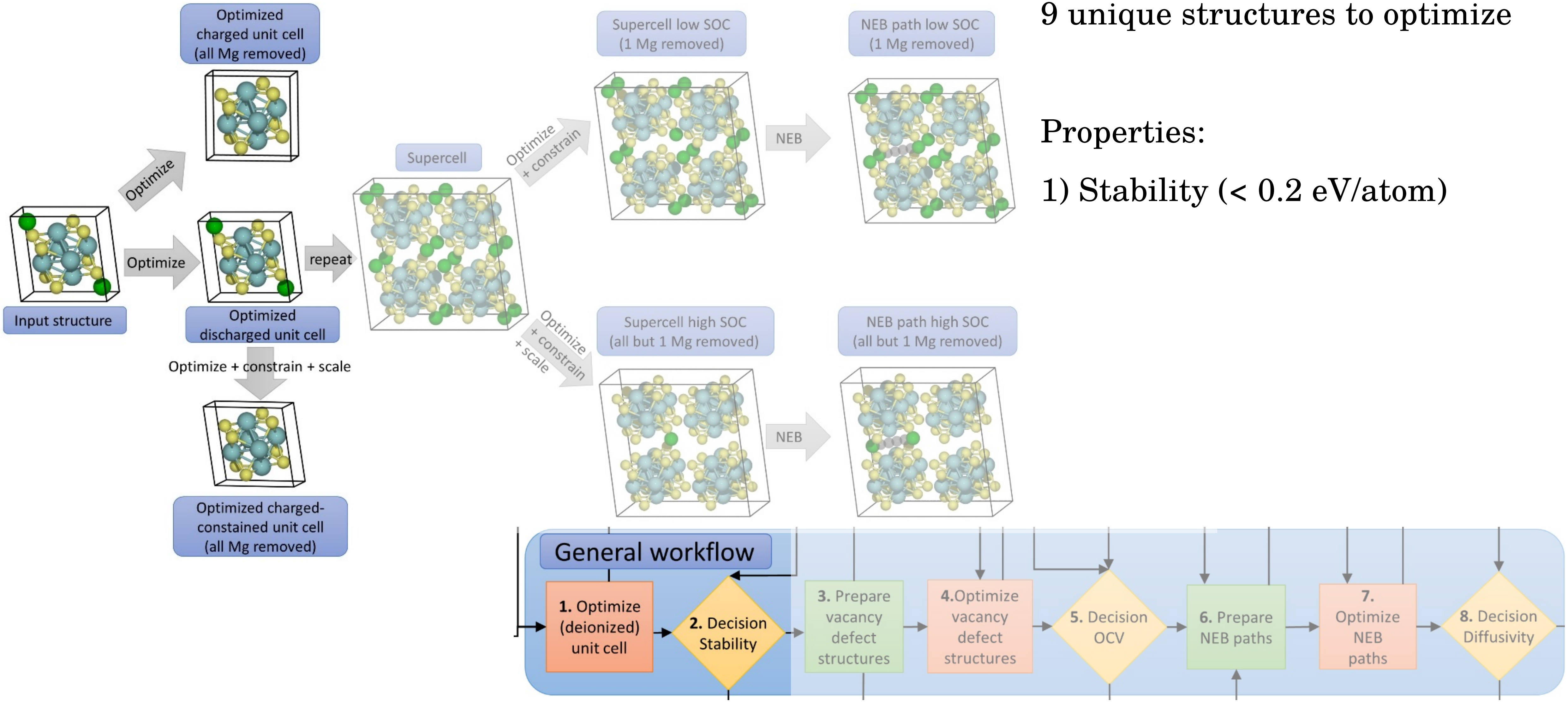


Bölle, Mathiesen, Nielsen, Vegge, Garcia Lastra, and Castelli, *BatteriesSupercaps* ***3**, 488* (2021)

Larsen *et al.*, *Journal of Physics: Condensed Matter* **29**, 27 (2017)

Mortensen *et al.*, *Journal of Open Source Software* **5**, 1844 (2020)

Preparation of the Structures



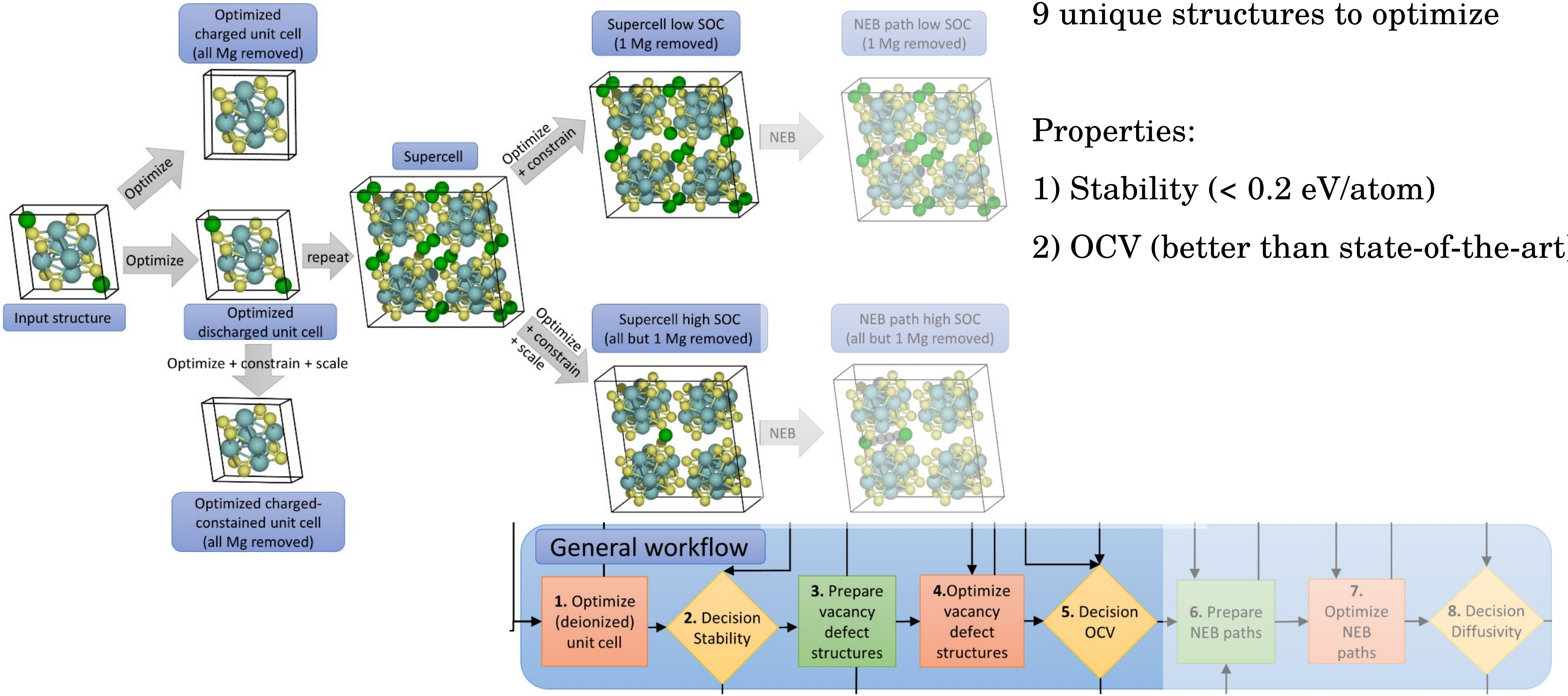
9 unique structures to optimize

Properties:

1) Stability (< 0.2 eV/atom)

Bölle, Mathiesen, Nielsen, Vegge, Garcia Lastra, and Castelli, *BatteriesSupercaps* ***3****, 488* (2021)

Preparation of the Structures



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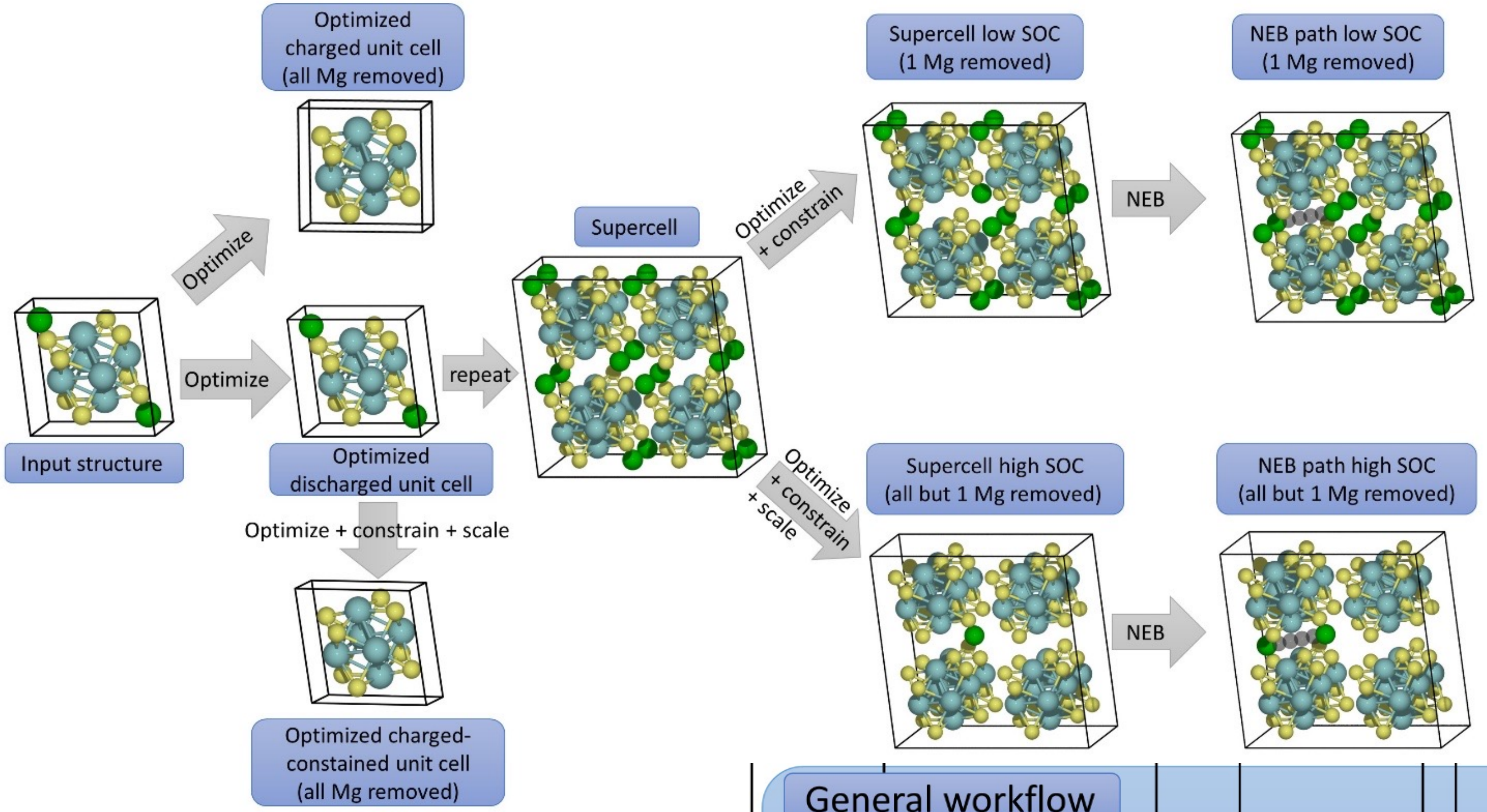
2) OCV (better than state-of-the-art)

Bölle, Mathiesen, Nielsen, Vegge, Garcia Lastra, and Castelli, *BatteriesSupercaps* ***3****, 488* (2021)

Preparation of the Structures



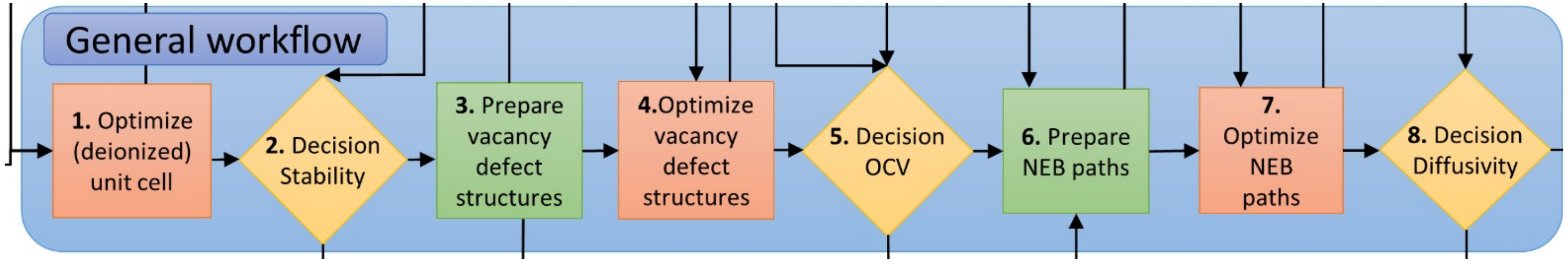
9 unique structures to optimize

Properties:

1) Stability (< 0.2 eV/atom)

2) OCV (better than state-of-the-art)

3) Diffusion (Nudged Elastic Bands Method, NEB)



Bölle, Mathiesen, Nielsen, Vegge, Garcia Lastra, and Castelli, *BatteriesSupercaps* ***3**, 488* (2021)

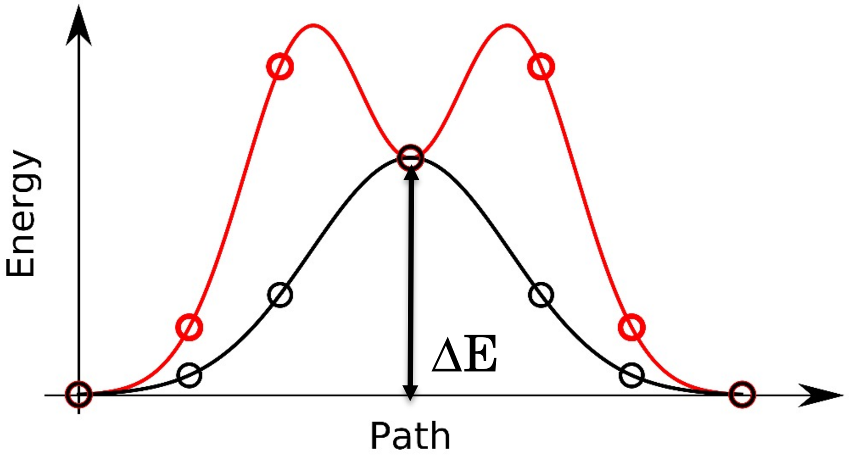
NEB Method

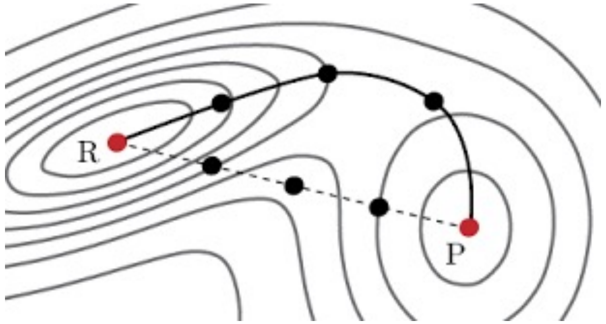
Find transition states and minimum energy paths between reactants (initial) and products (final)

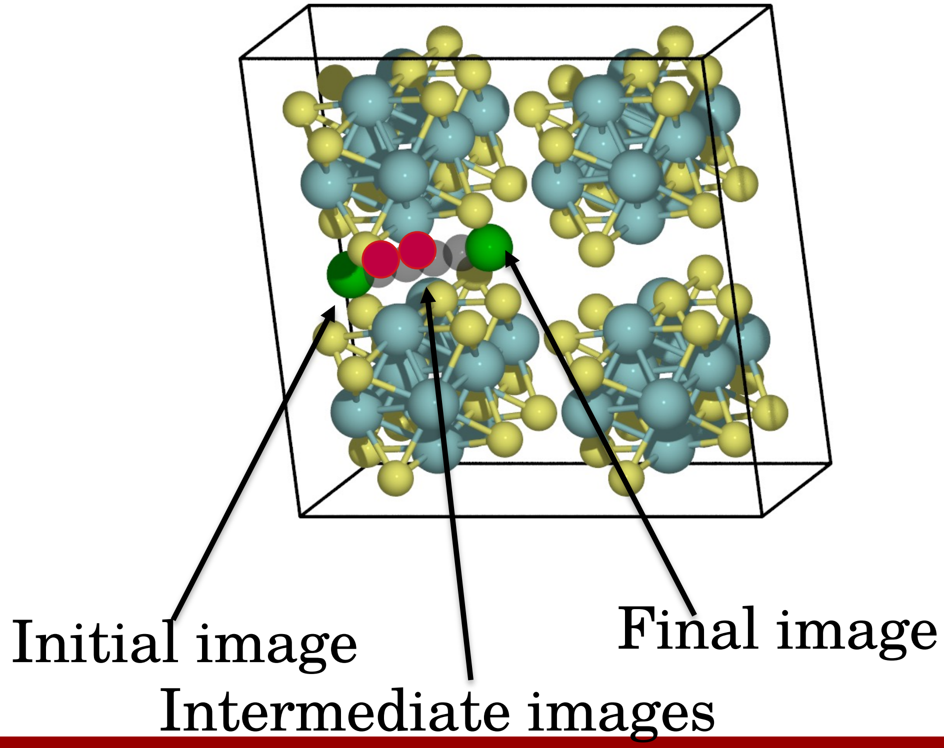
Expensive as many images needs to be calculated

Accelerated NEBs: use symmetries to reduce the number of images

Conventional NEB







Henkelman and Jonsson, *J. Chem. Phys.* **113**, 9978 (2000)

Mathiesen *et al.*, *Journal of chemical theory and computation* **15**, 3215 (2019)

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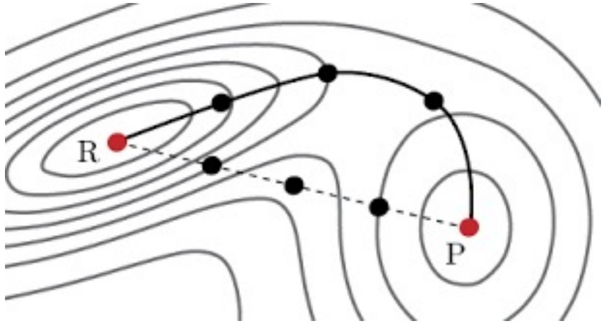
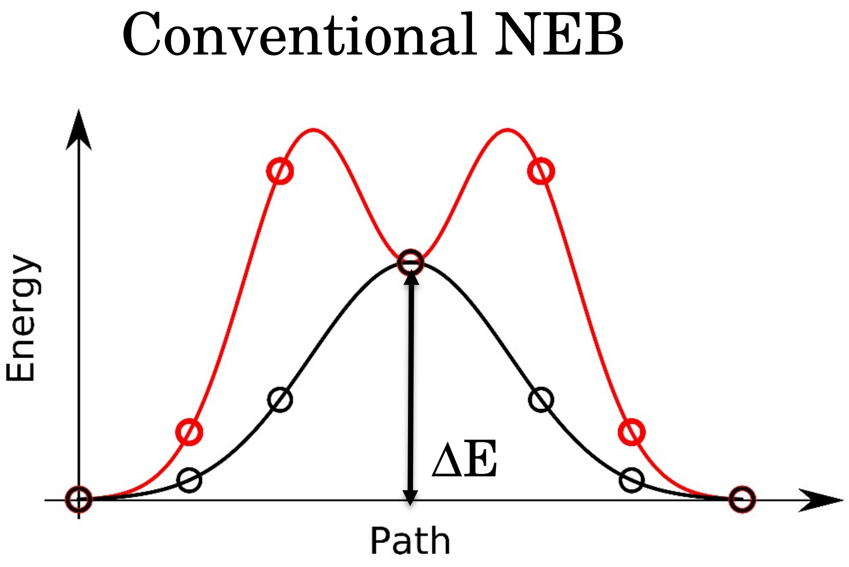
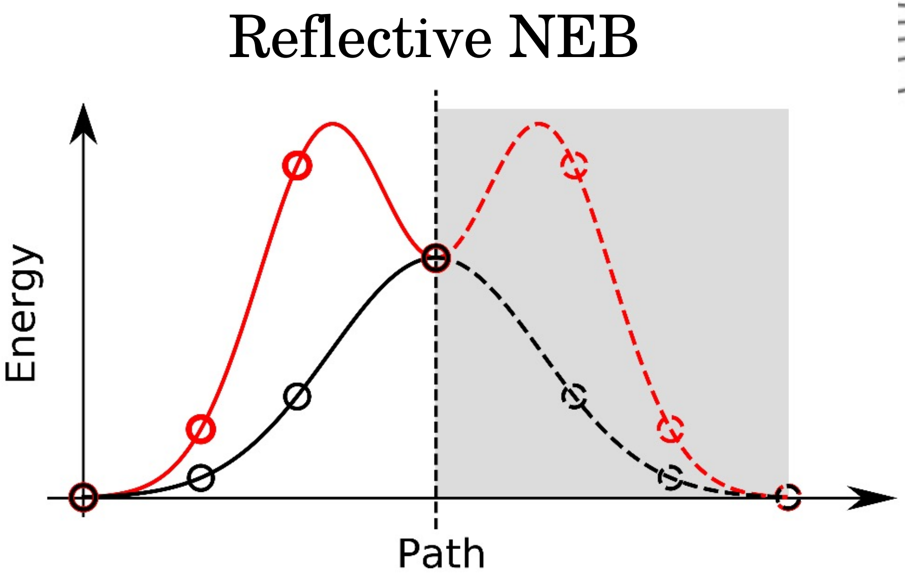
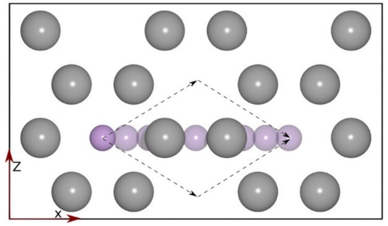
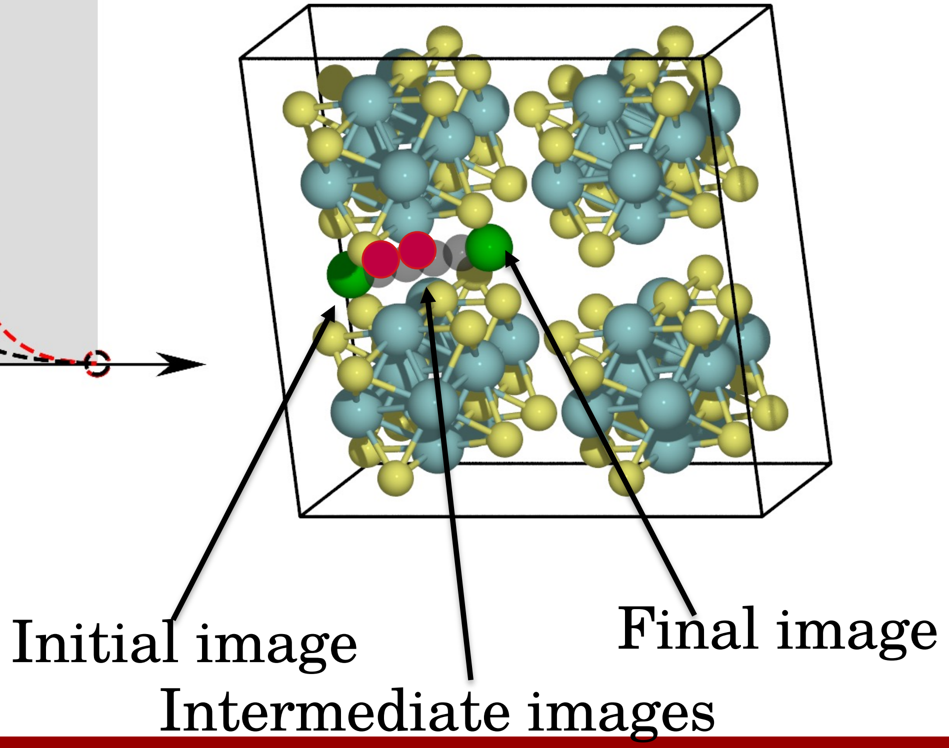




Speed-up: 2





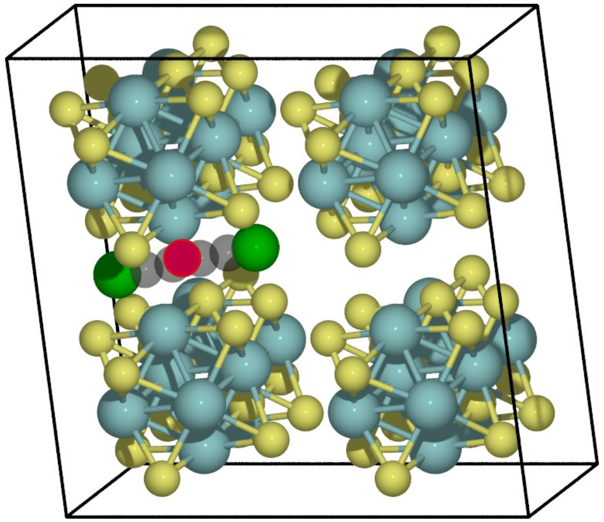


Henkelman and Jonsson, *J. Chem. Phys.* **113**, 9978 (2000)

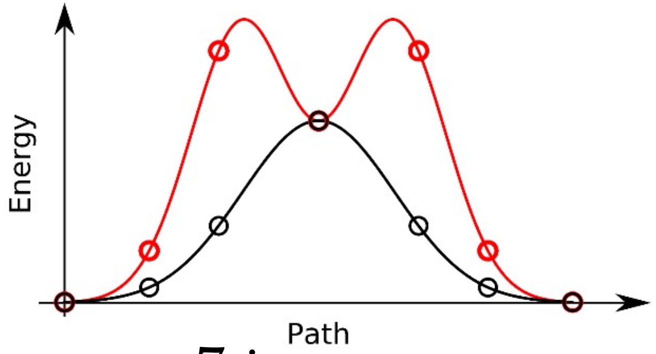
Mathiesen *et al.*, *Journal of chemical theory and computation* **15**, 3215 (2019)

Accelerated NEBs

Climbing image (find transition state)

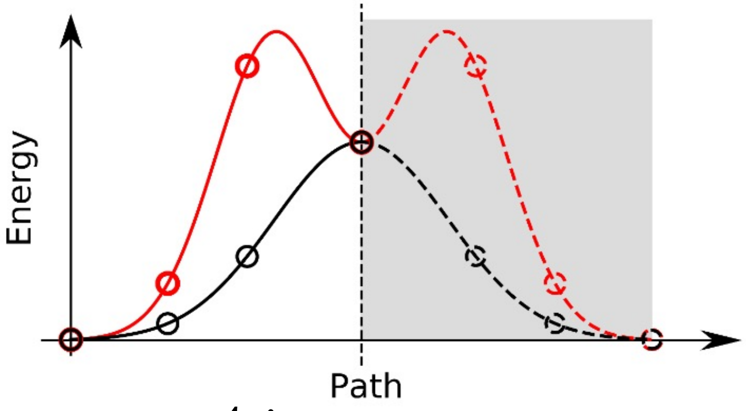


Conventional NEB



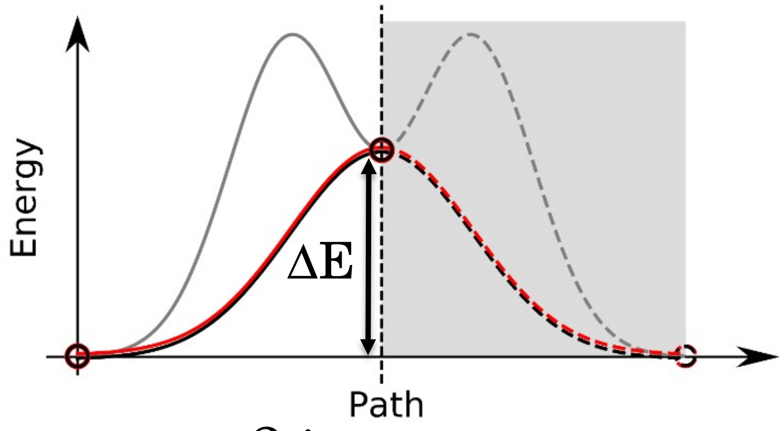
7 images

Reflective NEB (RNEB)



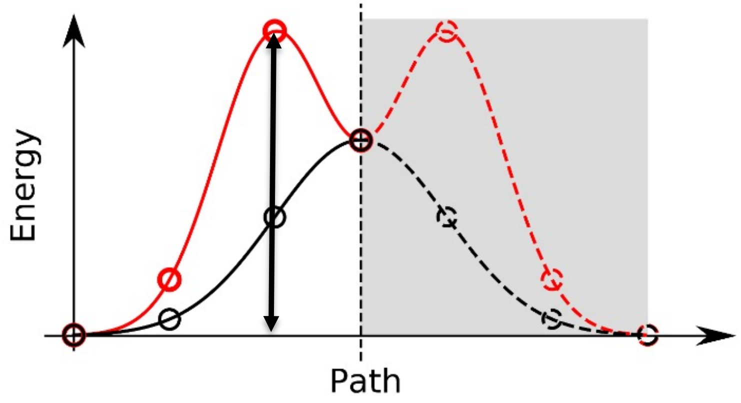
4 images

Reflective middle-image (RMI) NEB



2 images

Climbing image RNEB

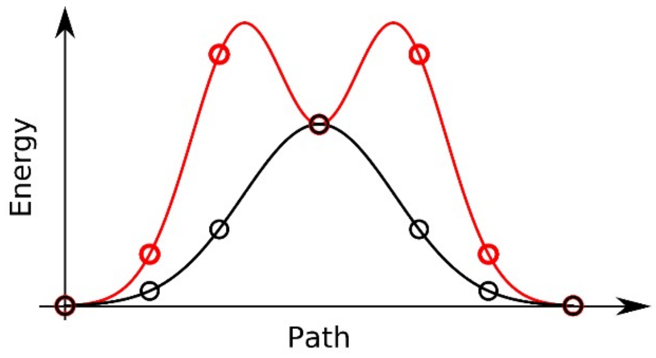


4 images

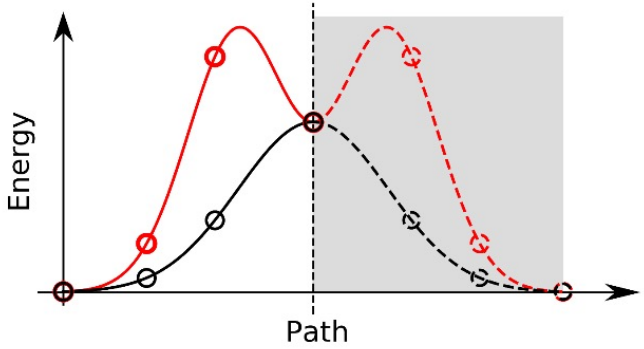
Henkelman and Jonsson, *J. Chem. Phys.* **113**, 9978 (2000); Mathiesen *et al.*, *Journal of chemical theory and computation* **15**, 3215 (2019)

Accelerated NEBs – in the Workflow

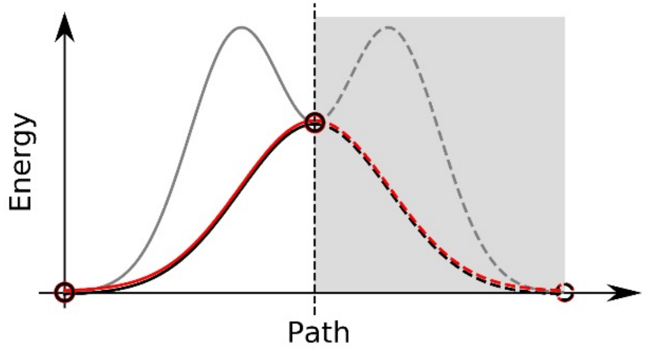
Conventional NEB



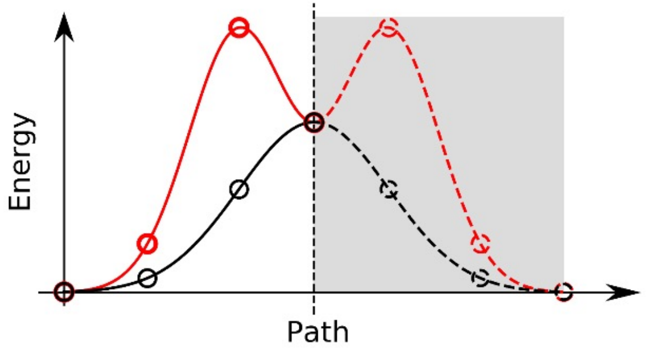
RNEB

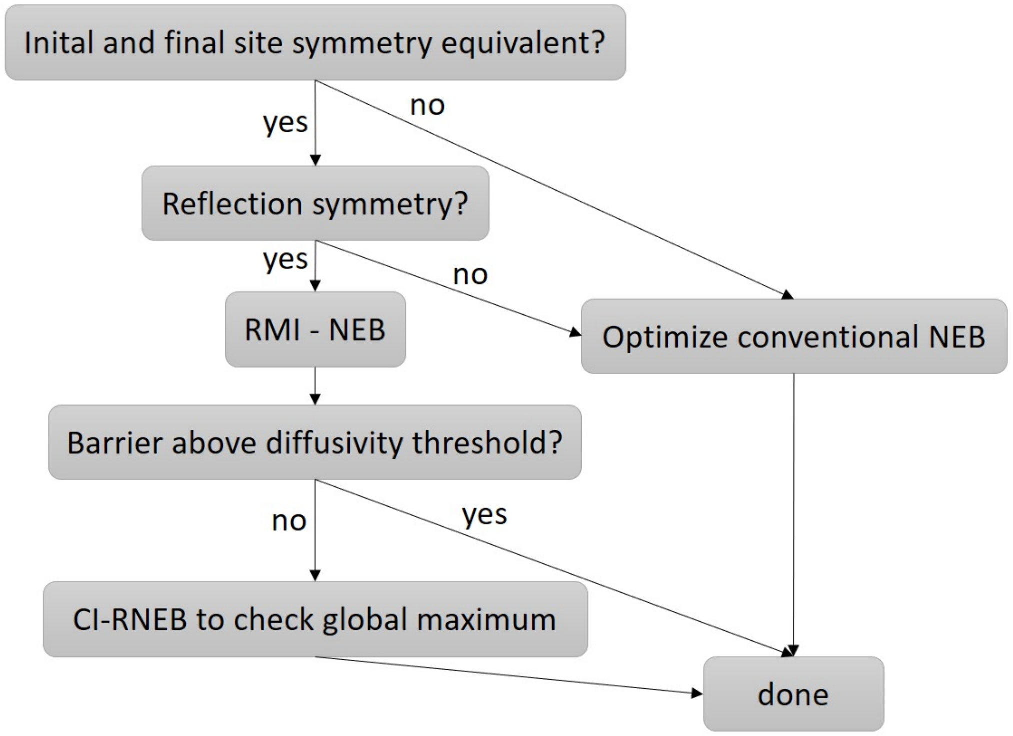


RMI - NEB



CI - RNEB





CAN WE ACCELERATE THIS EVEN FURTHER????

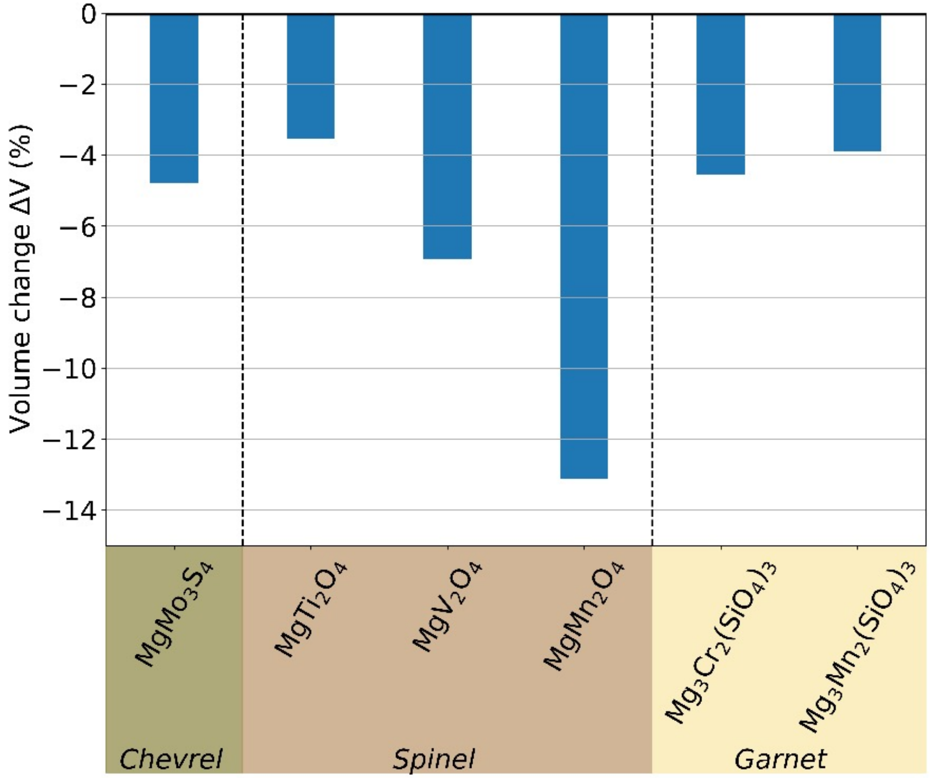
More details: Bölle – Wed 17th, 11.50

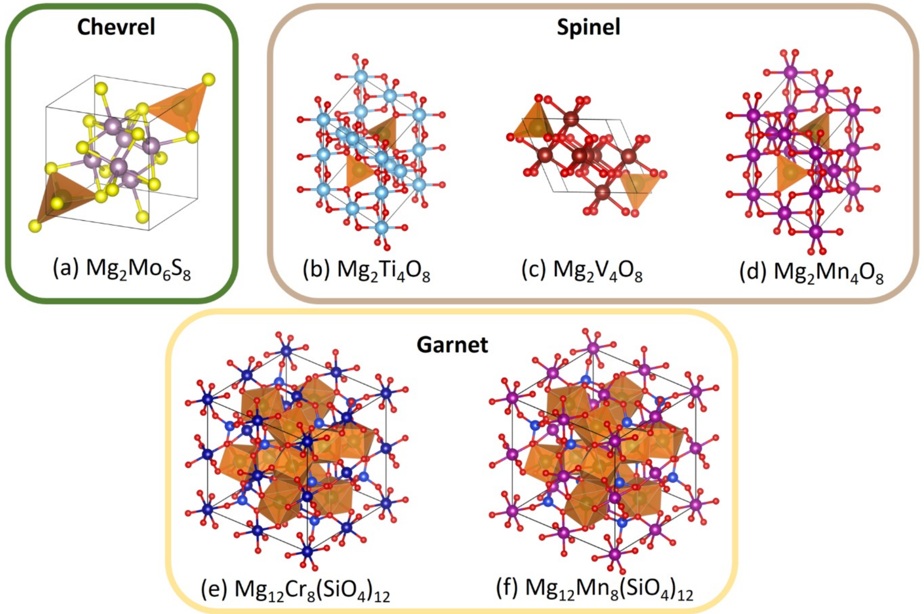
Bölle, Mathiesen, Nielsen, Vegge, Garcia Lastra, and Castelli, *BatteriesSupercaps* ***3****, 488* (2021)

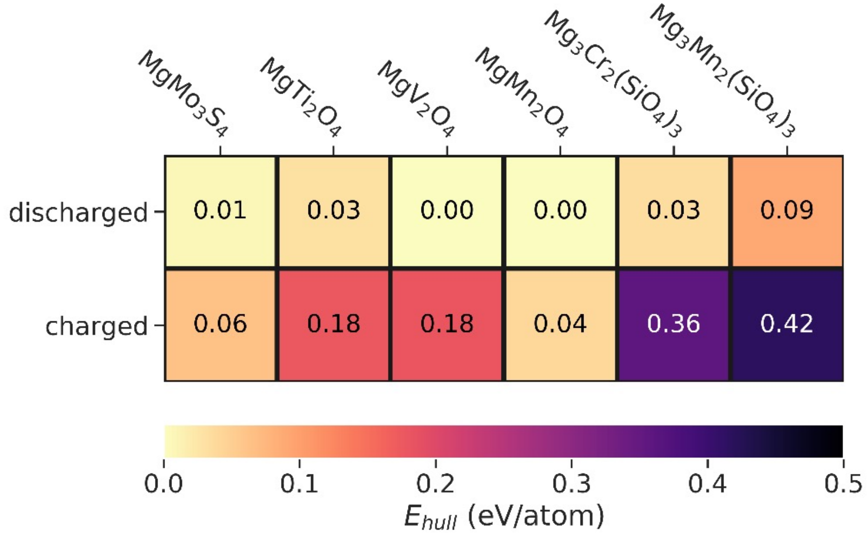
Candidate Materials from the ICSD Database

~100 Materials from the ICSD database

1) stability and volume change





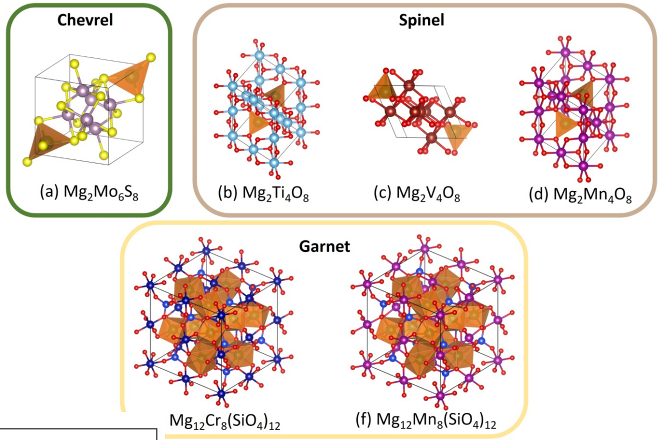


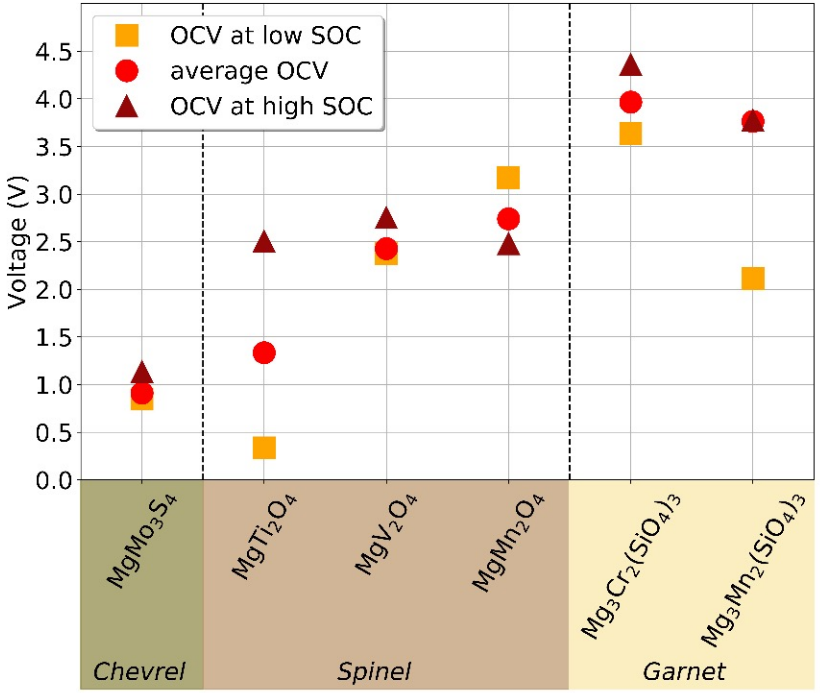
Bölle, Mathiesen, Nielsen, Vegge, Garcia Lastra, and Castelli, *BatteriesSupercaps* ***3****, 488* (2021)

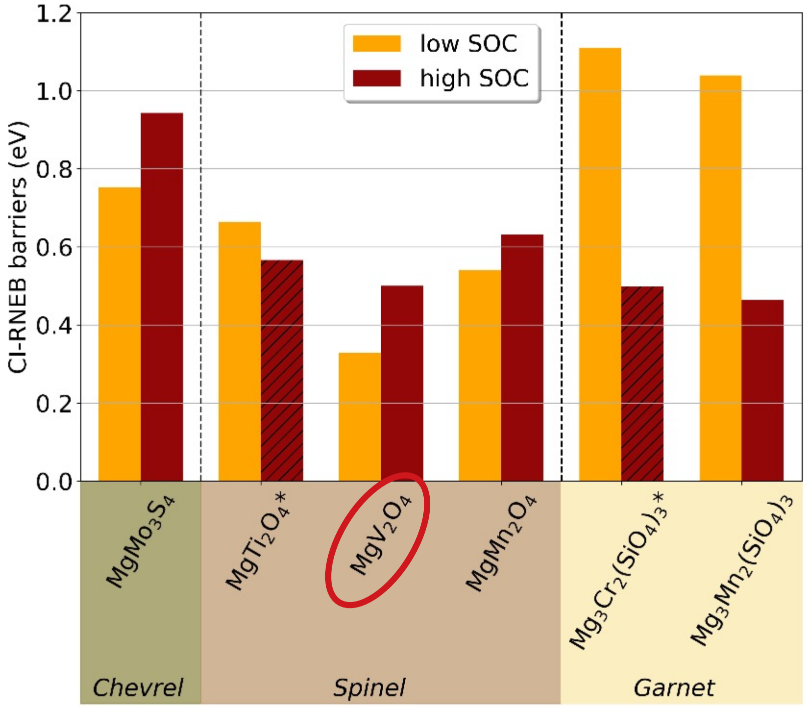
Candidate Materials from the ICSD Database

~100 Materials from the ICSD database

1) stability and volume change
2) OCVs
3) Diffusion Barriers





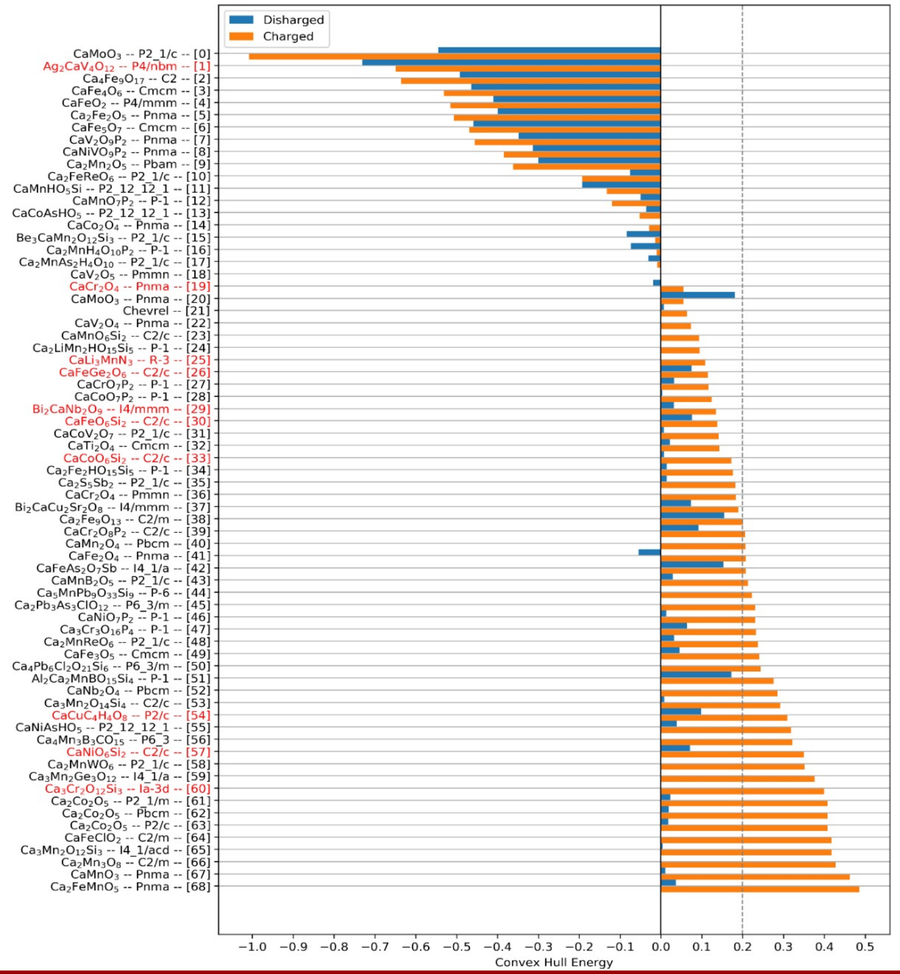


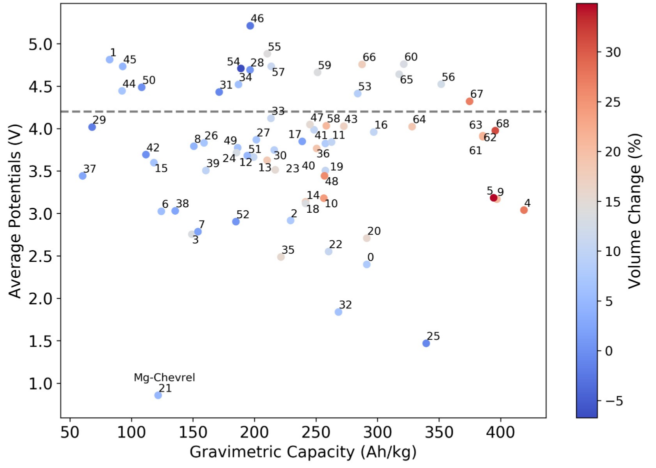
Bölle, Mathiesen, Nielsen, Vegge, Garcia Lastra, and Castelli, *BatteriesSupercaps* ***3****, 488* (2021)

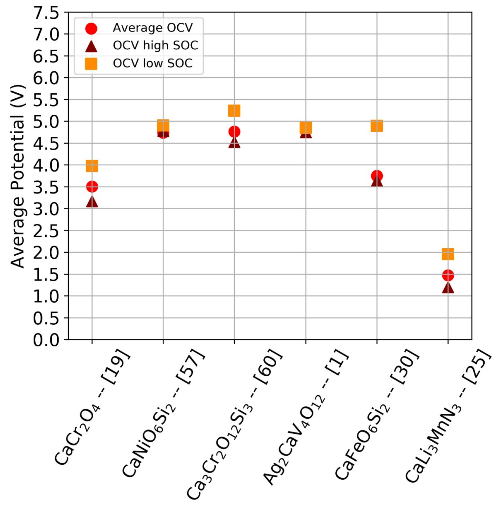
Re-use the Workflow: Ca-ion Batteries

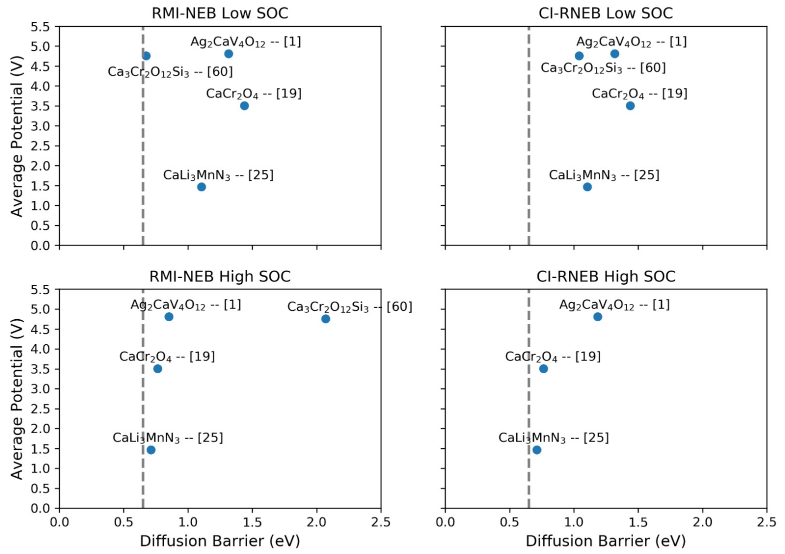
Abundance, multivalent ion, redox potential

~250 Materials from the ICSD database



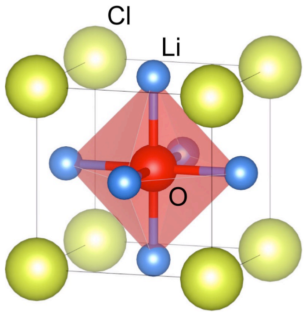






Re-use the Workflow: Antiperovskites for Solid-State Batteries

Higher capacity and safer devices – Limitations: low conductivity



Antiperovskites (Li_3BrO, Li_3ClO,…)

1) **Electronic conduction**
- Large band gaps

2) **Ionic conductivity**
- High ionic conductivity

3) **Stability:**
- Stability against lithium-metal anode
- Li_3BrO and Li_3ClO stable vs Li/Li^+ redox potential
- Often unstable in water

4) **Mechanical properties**
- Resistance to dendrite penetration

5) **Sustainability**
- It can accommodate diverse elements (Li, Na mostly synthetized)

Re-use the Workflow: Antiperovskites for Solid-State Batteries

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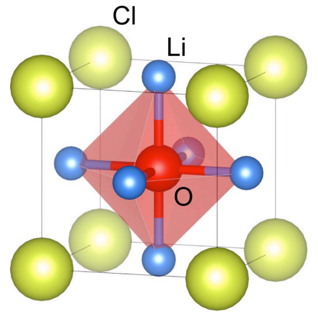

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4) **Mechanical properties**
- Resistance to dendrite penetration

5) **Sustainability**
- It can accommodate diverse elements (Li, Na mostly synthetized)

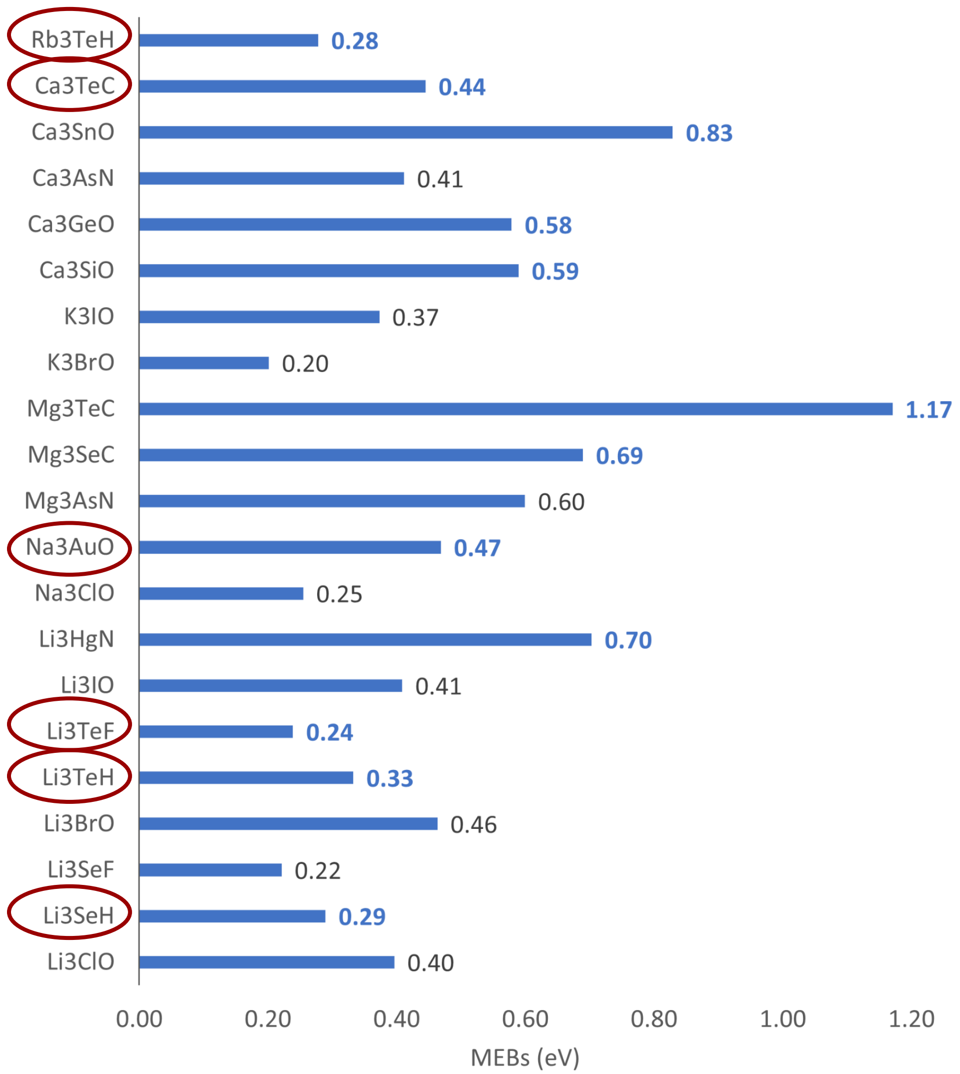
Database-based selection:
- Geometric filter
- Band gap value
- Sustainability constituent elements

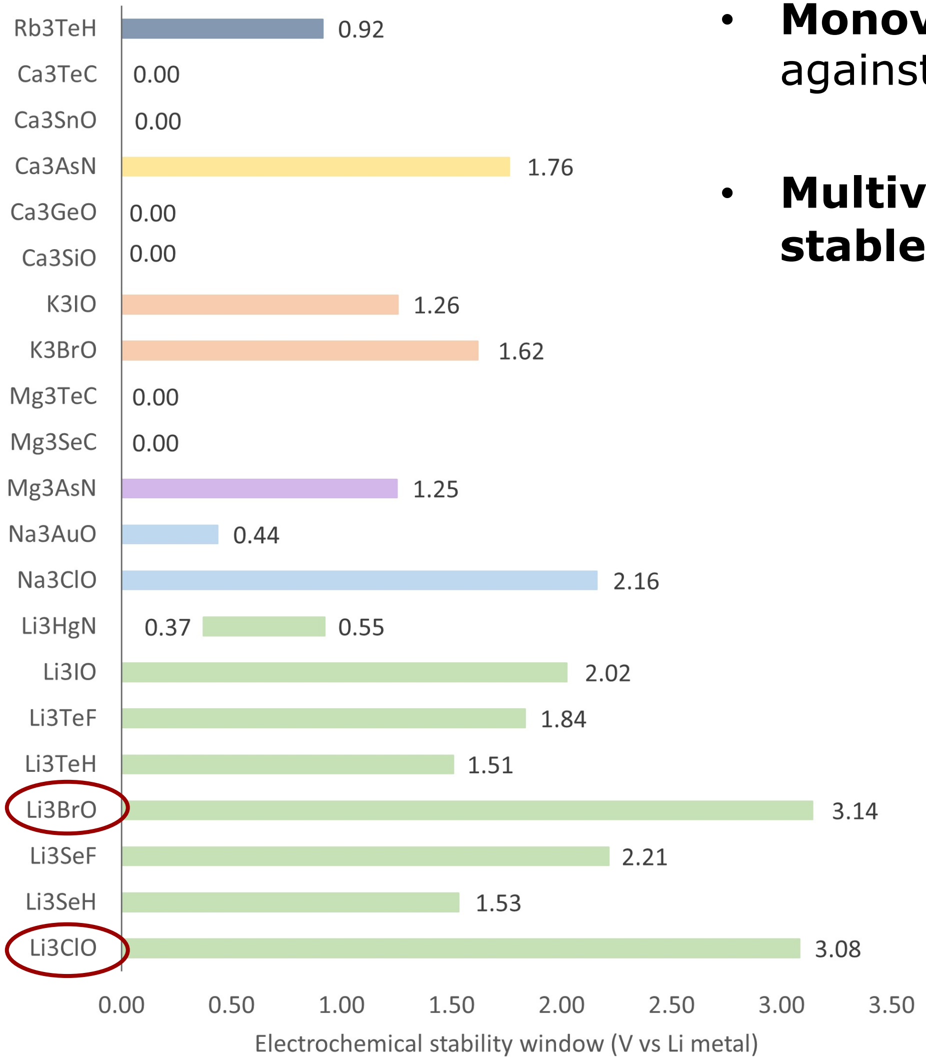
Thermodynamic stability:
- Energy above the convex hull

Ionic Conductivity:
- Migration energy barriers (NEB methods within DFT)

Stability under operating conditions:
- Real band gap
- Stability with moisture
- Electrochemical stability window vs metal anode

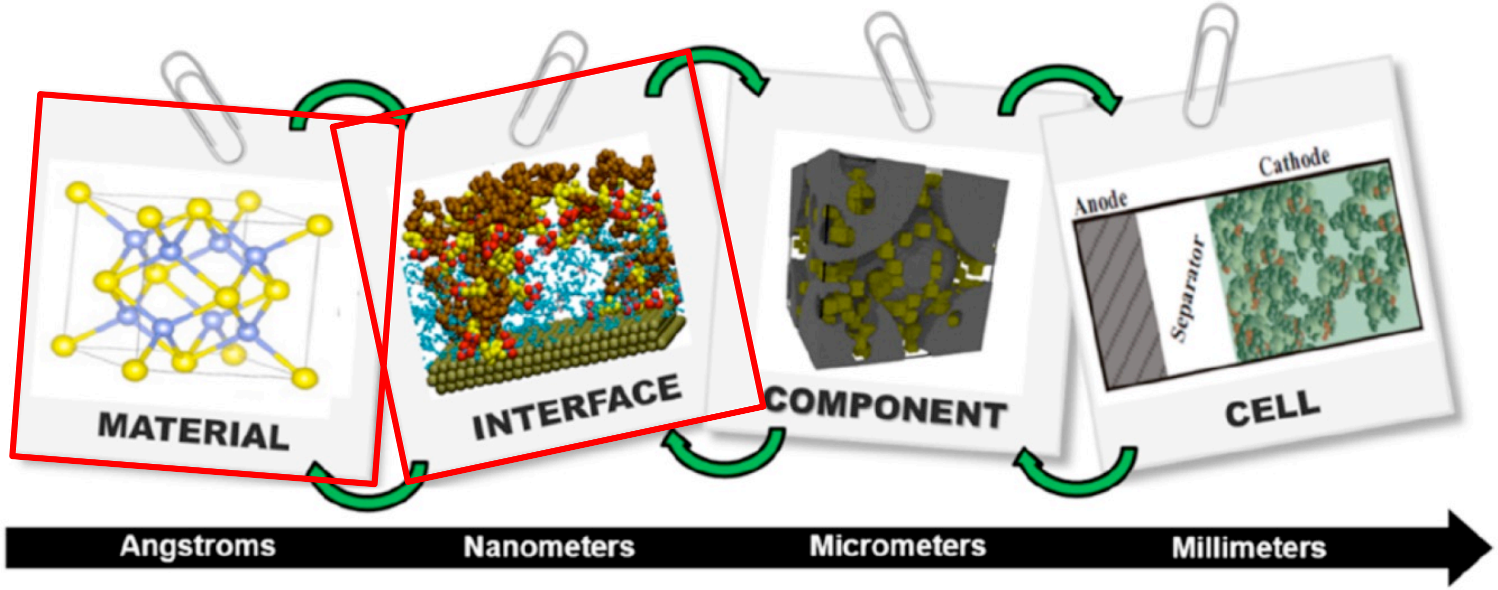
Migration Barriers and Electrochemical Stability



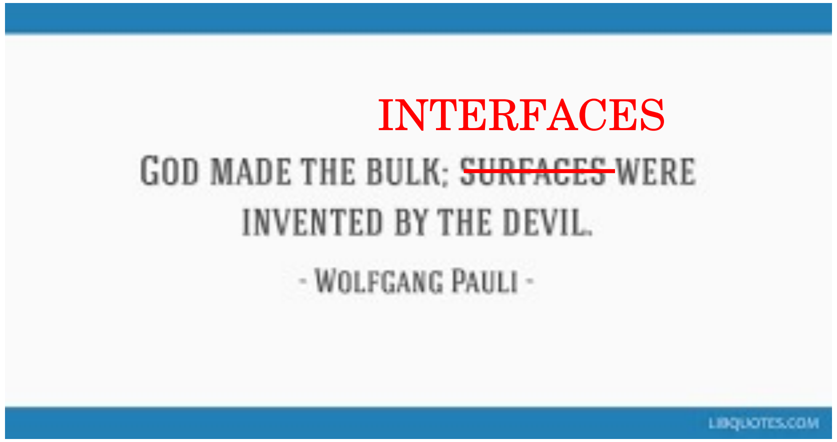


- **Monovalent cation stable** against cation-metal
- **Multivalent cation less stable** against metal

Can We Implement Workflows for Interfaces?



Franco *et al.*, *Chem. Rev.* **119**, 4569 (2019)



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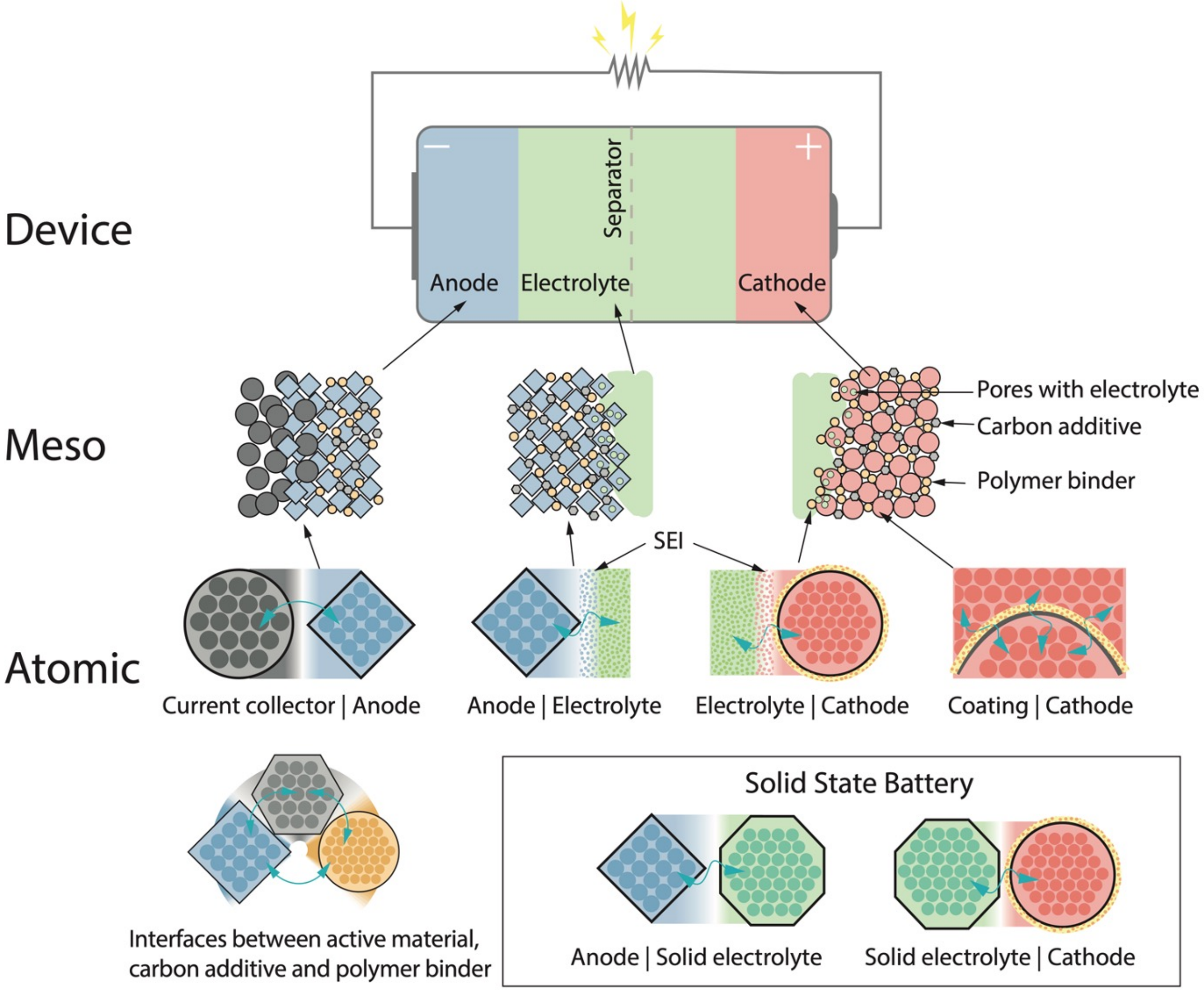
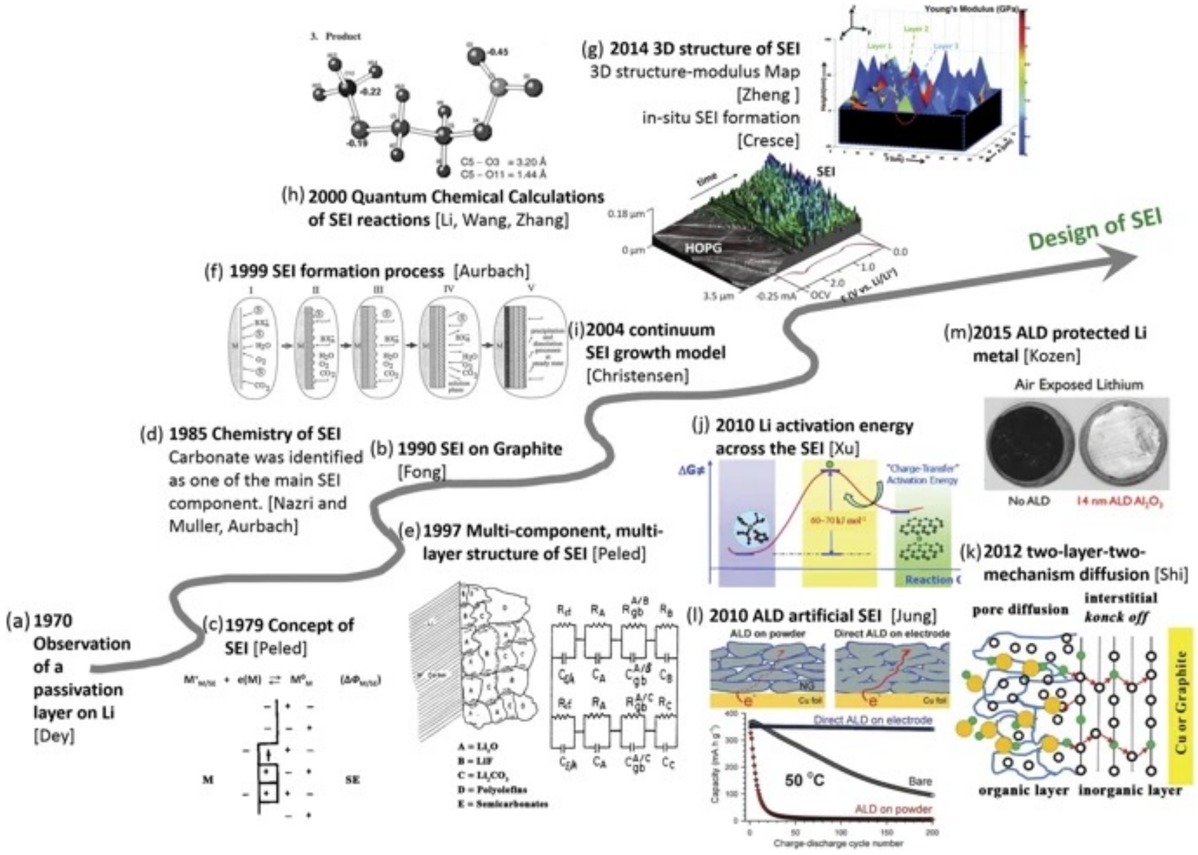
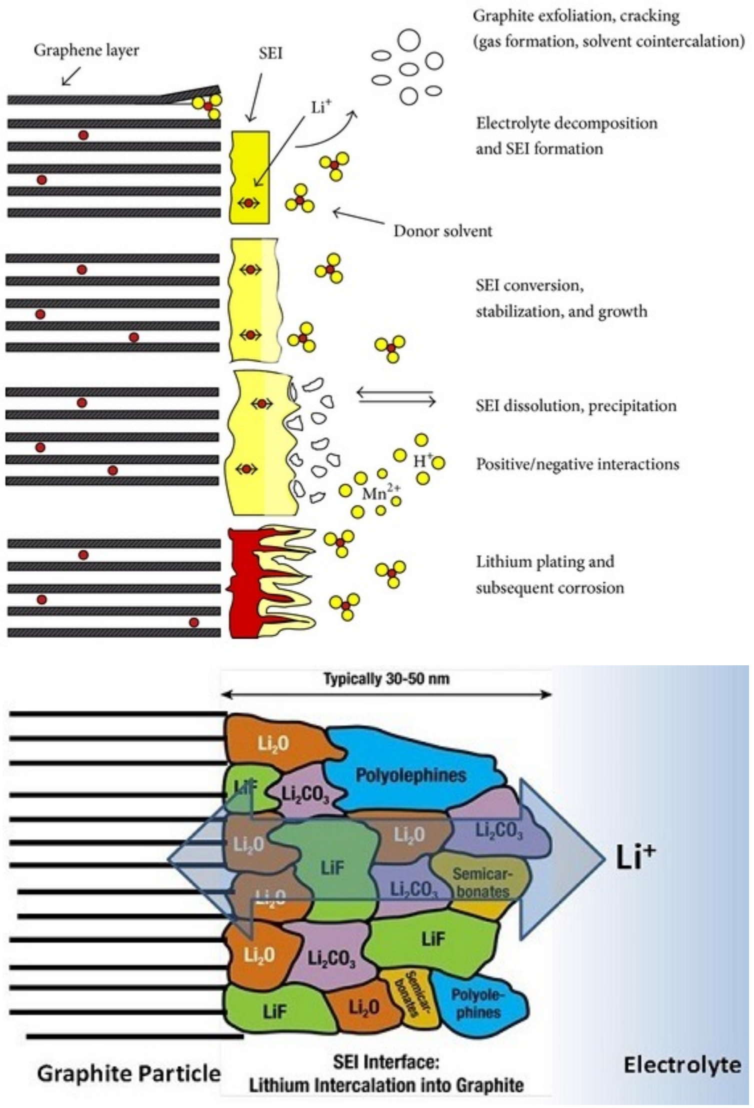


	Entries	App	Battery	Workflow	API
Materials Project – https://www.materialsproject.org/ – Provenance: USA					
	Entries	**App**	**Battery**	**Workflow**	**API**
Total Entries	711,561	Phase Diagram	–	Fireworks Automate Pymatgen Custodian	YES
Intercalation Electrodes	4,730	Reaction Calculator	YES		
Conversion Electrodes	16,128	Battery explorer			
Liquid Electrolytes	49,705	Explore Molecule Redox Flow Batteries	YES		
Bulk Interfacial Reactivity	N.A.	Interface Reaction (Bulk)	YES		
The Open Quantum Materials Database – OQMD – http://oqmd.org – Provenance: USA					
Total entries	815,654	Phase Diagram	NO	OQMD	YES
Automatic FLOW for Materials Discovery – http://www.aflowlib.org – Provenance: USA					
Total entries	3,482,348	Phase Diagram (AFLOW-Chull)	NO	AFLOW	YES
Novel Materials Discovery – NOMAD – https://nomad-lab.eu/ – Provenance: Germany/EU					
Total entries	>11,000,000	Artificial Intelligence Toolkit	NO	Qmpy	YES
Materials Cloud – https://www.materialscloud.org – Provenance: Switzerland/EU					
Total entries	7,502,686	–	YES	AiiDA	YES
BIG-MAP App Store – https://big-map.github.io/big-map-registry – Provenance: Denmark/EU					
Total entries	N.A.	BattINFO DFT-Surface	YES	AiiDA SimStack	YES
ARTISTIC Computational Portal – https://www.erc-artistic.eu/computational-portal – Provenance: France/EU					
Total entries	>111 (open since July 2021)	Online Manufacturing Simulator Data Explorer INNOV	YES	ARTISTIC	NO

Deng, Kumar, Bölle, Caro, Franco, Castelli, Canepa, Seh, under review (2021)

The Case of the Solid Electrolyte Interphase





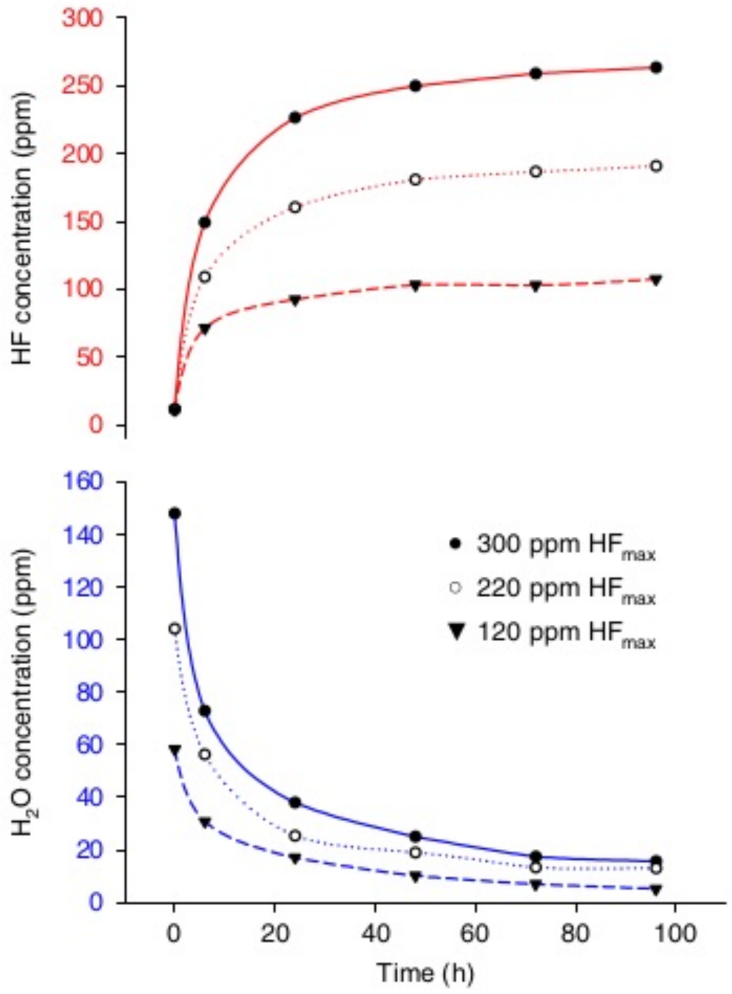
Winter, *Zeitschrift für Physikalische Chemie* **223**, 1395 (2009)

Dunn, Kamath, and Tarascon, *Science* **334**, 928 (2011)

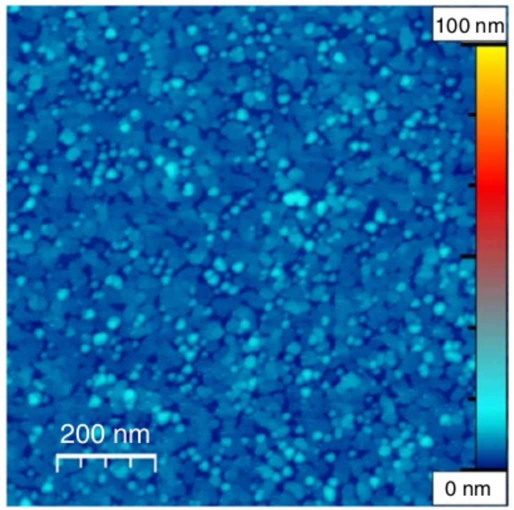
Lin, Tang, Mu, Wang, and Wang, *Journal of Chemistry* **2015**, 1 (2015)

Wang, Kadam, Li, Shi, and Qi, *npj Computational Materials* **4**, 15 (2018)

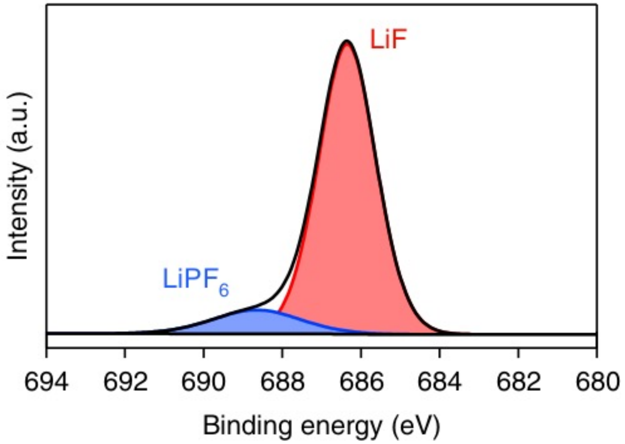
The SEI Formation on Metal Single Crystals



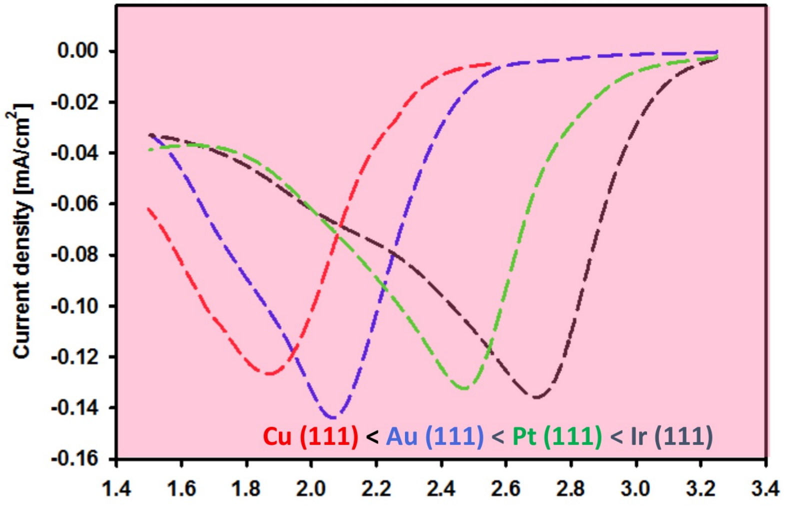
AFM: LiF@Au(111)

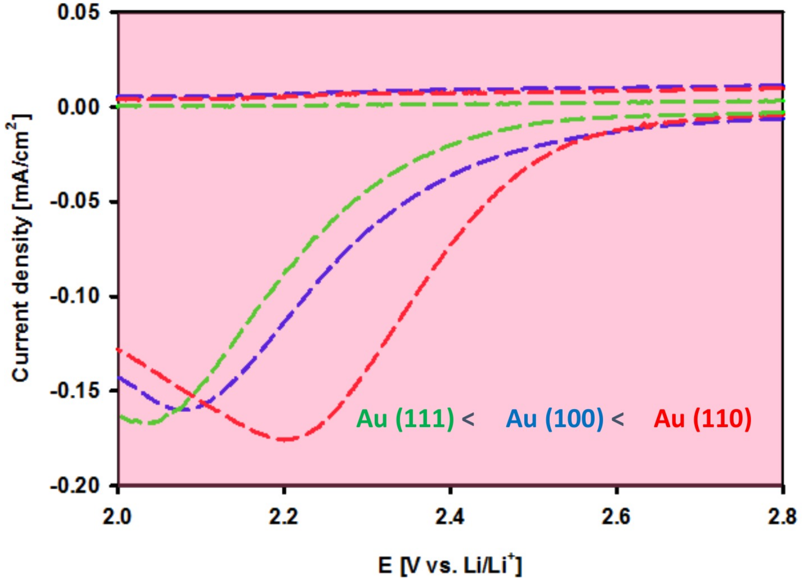


XPS



CV



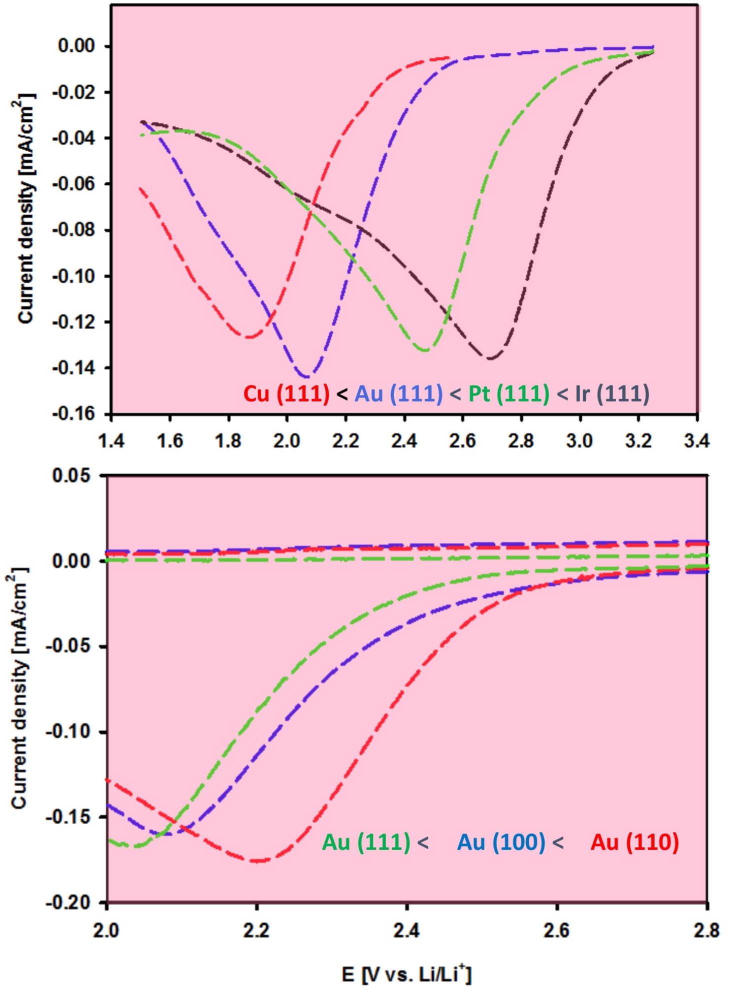


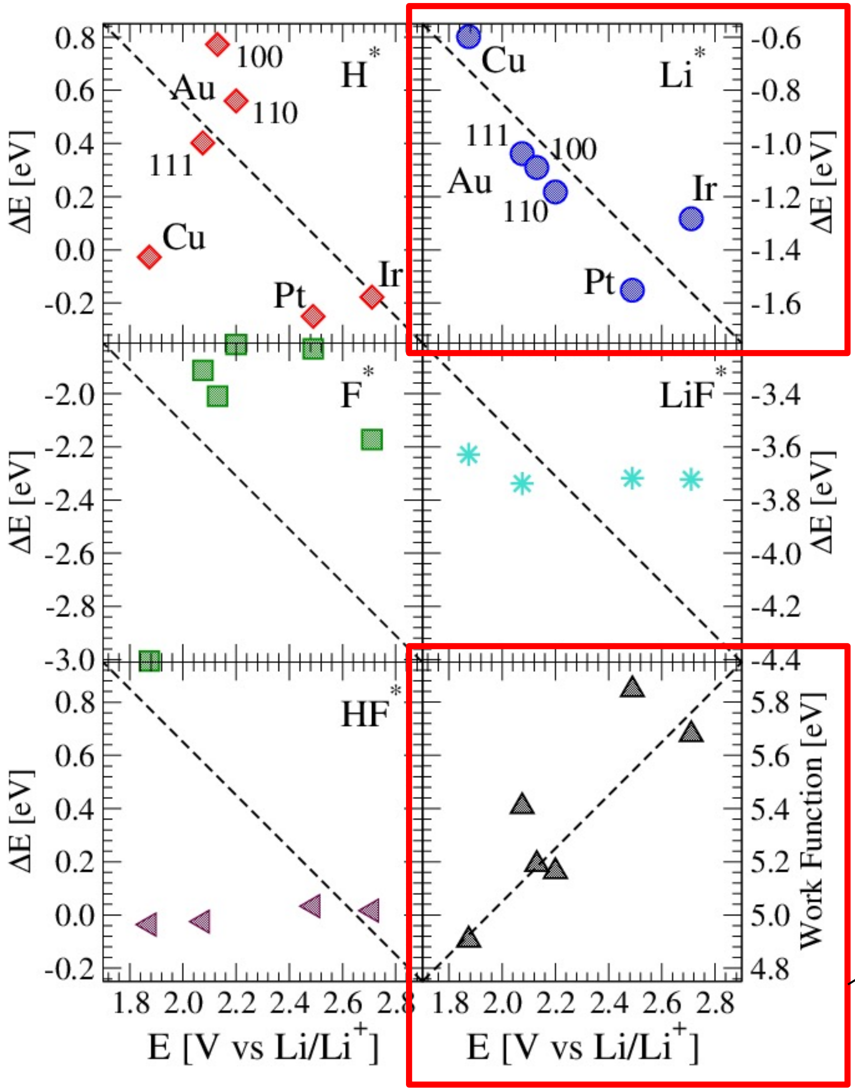
Electrolyte EC:EMC 3:7w (LP57)

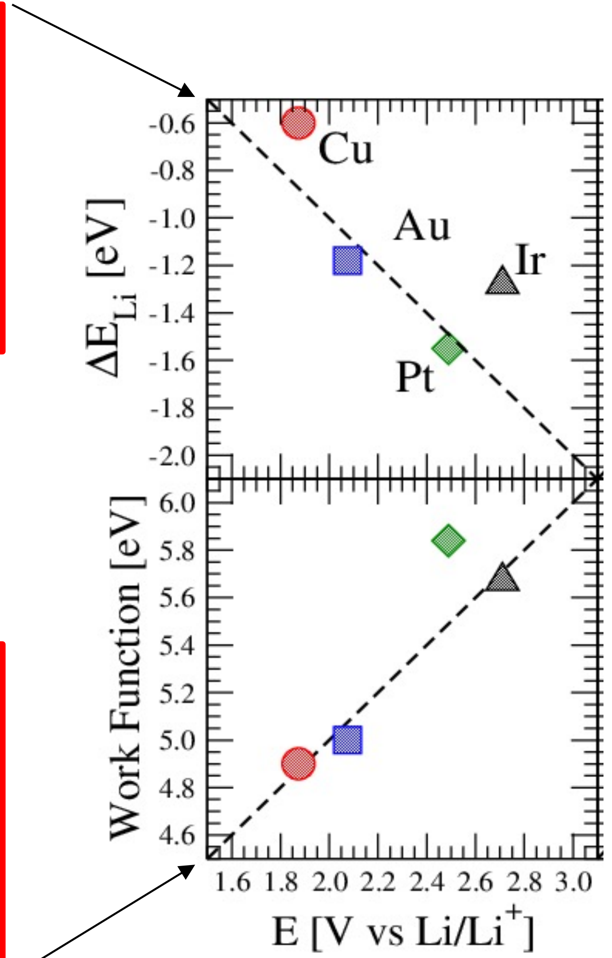
Only impurity: HF

Strmcnik, Castelli, …, Rossmeisl, and Markovic, *Nature Catalysis* **1**, 255 (2018)

Possible Descriptors







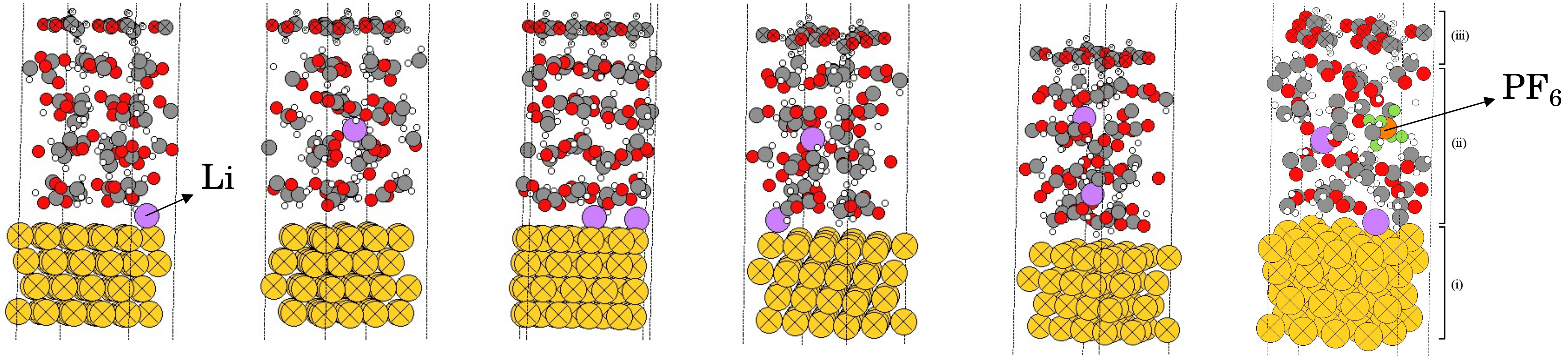
What is the role played by Li and by the interface?

Strmcnik, Castelli, …, Rossmeisl, and Markovic, *Nature Catalysis* **1**, 255 (2018)

Explicit Modelling of the Solid/Electrolyte Interface

Combination of *molecular dynamics* and *DFT* (Ab-initio MD, AIMD)

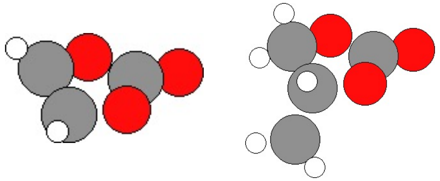
Study of the phase diagram of LP57 (EC:EMC 3:7w) with Li-atoms



Li coverages: 0 – 3 /16

Counter anion: PF_6

Additives: VC, PC, …



Castelli, Zorko, …, Strmcnik, and Rossmeisl, *Chem. Sci.* **11**, 3914 (2020)

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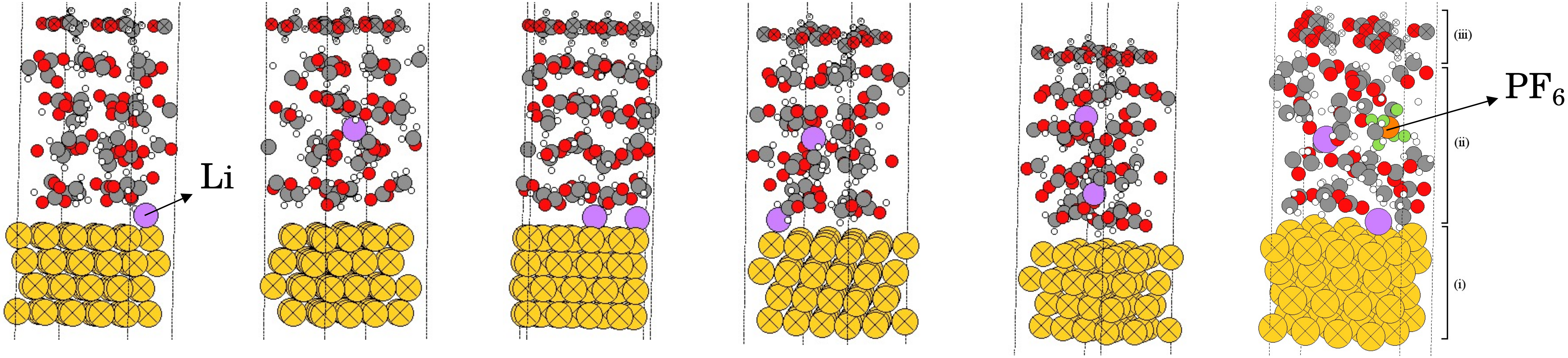

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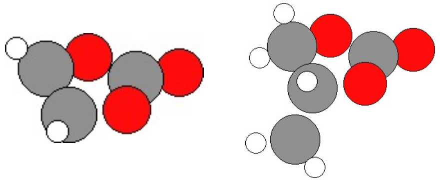

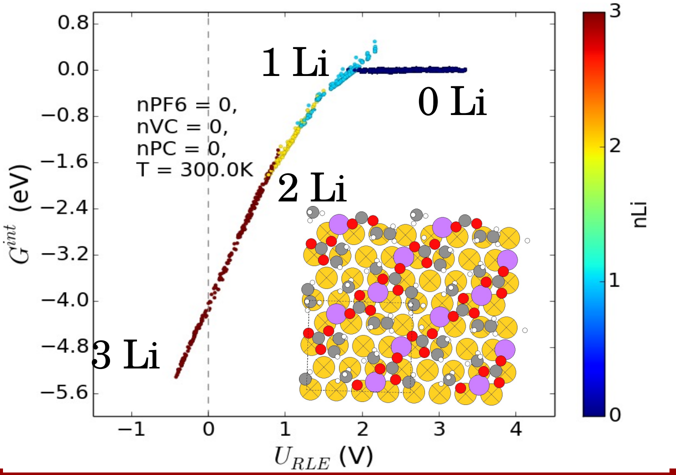

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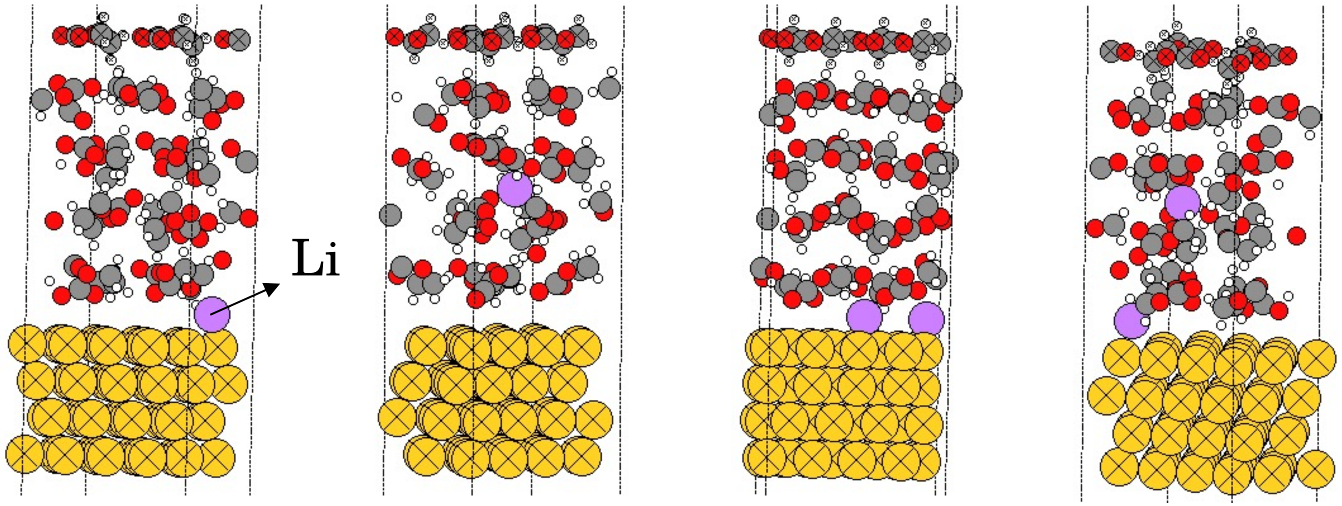

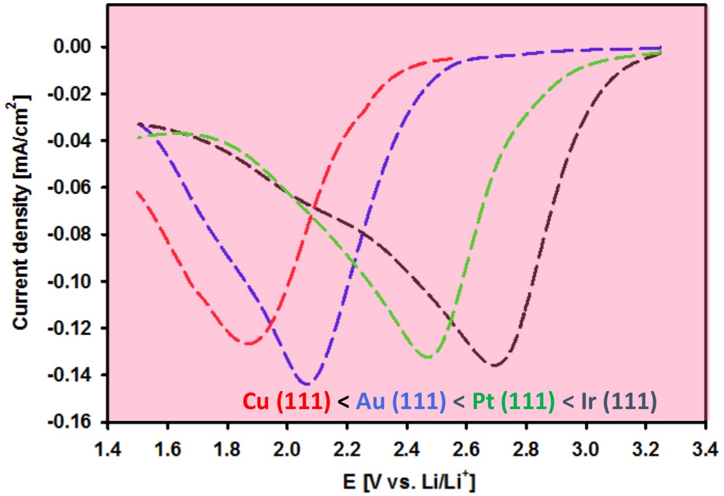

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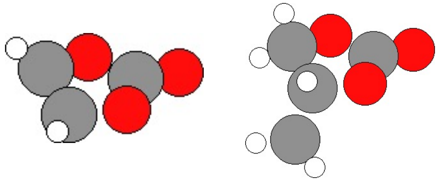
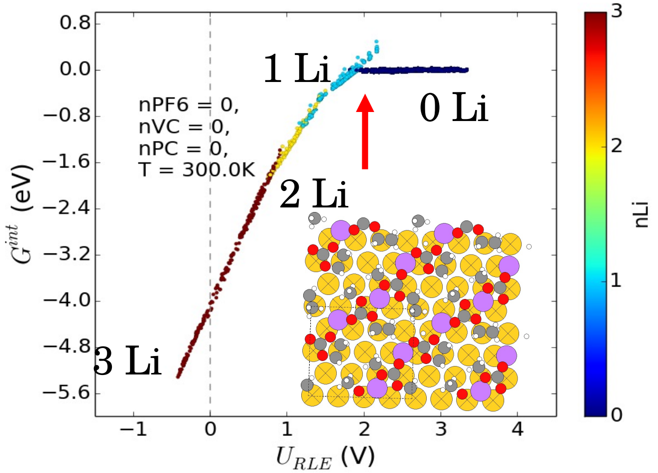
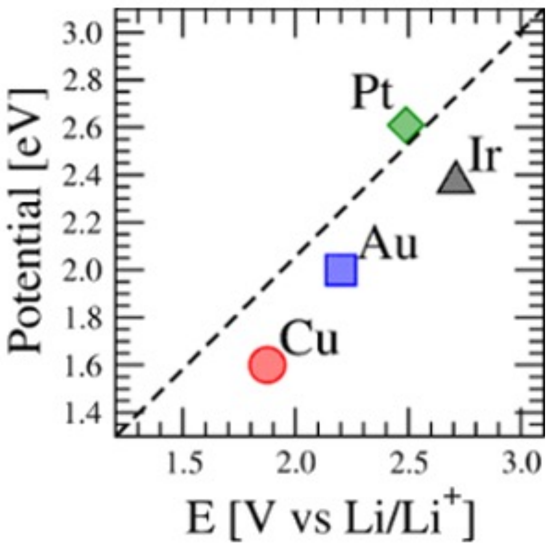




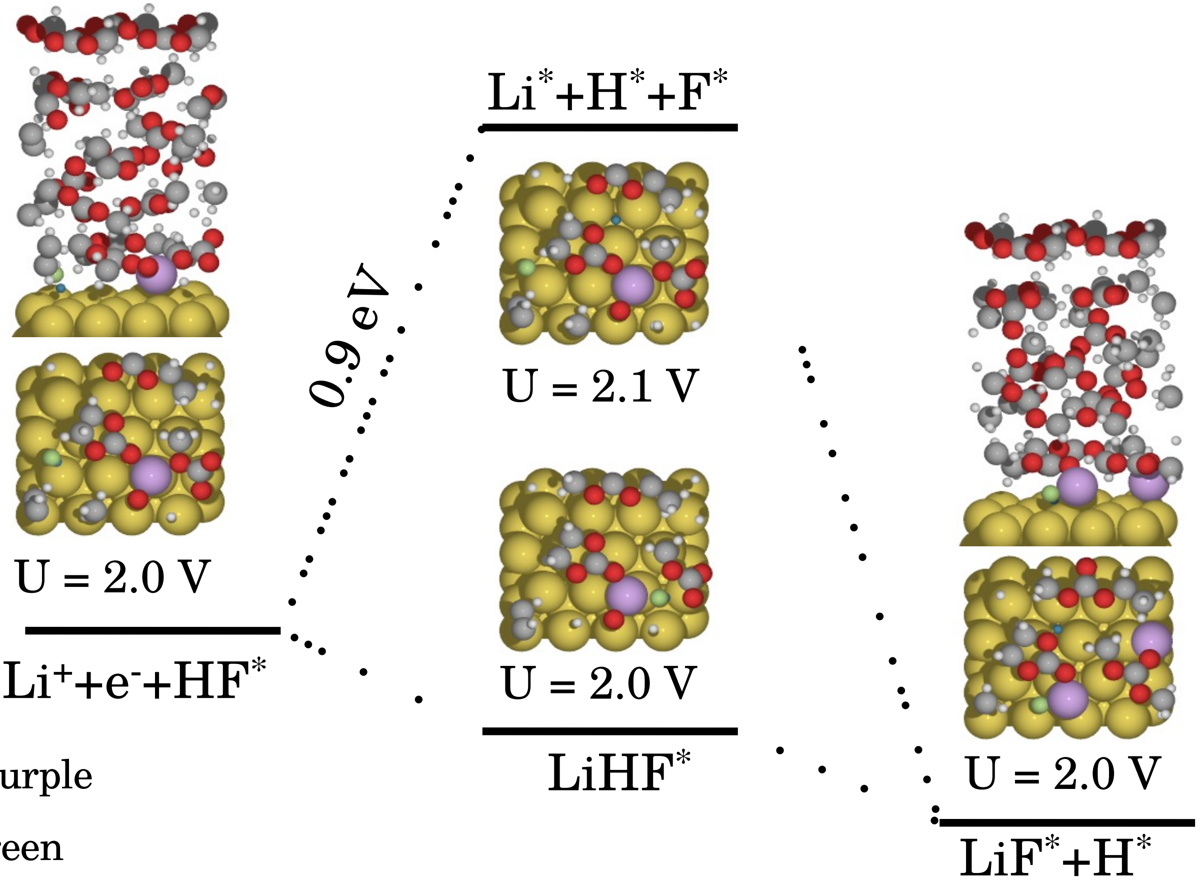
Li-adsorption Potential



Castelli, Zorko, …, Strmcnik, and Rossmeisl, *Chem. Sci.* **11**, 3914 (2020)

Reaction Paths on Au(111) in LP57

Note: the potential should be kept constant during the reaction and equal to the Li- adsorption potential!



Li = purple

F = green

H = white and blue (from HF)

O = red

C = gray

Au = yellow

Strmcnik, Castelli, …, Rossmeisl, and Markovic, *Nature Catalysis* **1**, 255 (2018)

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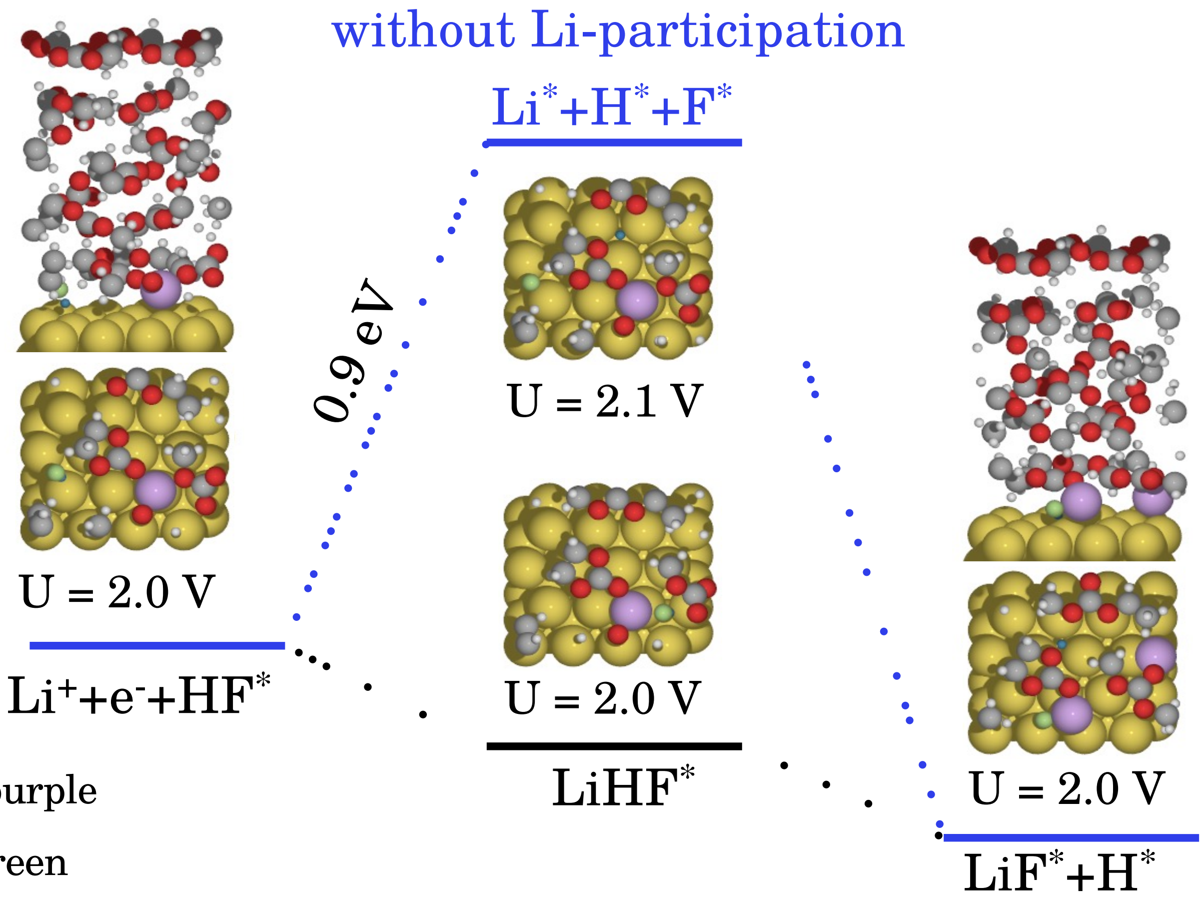

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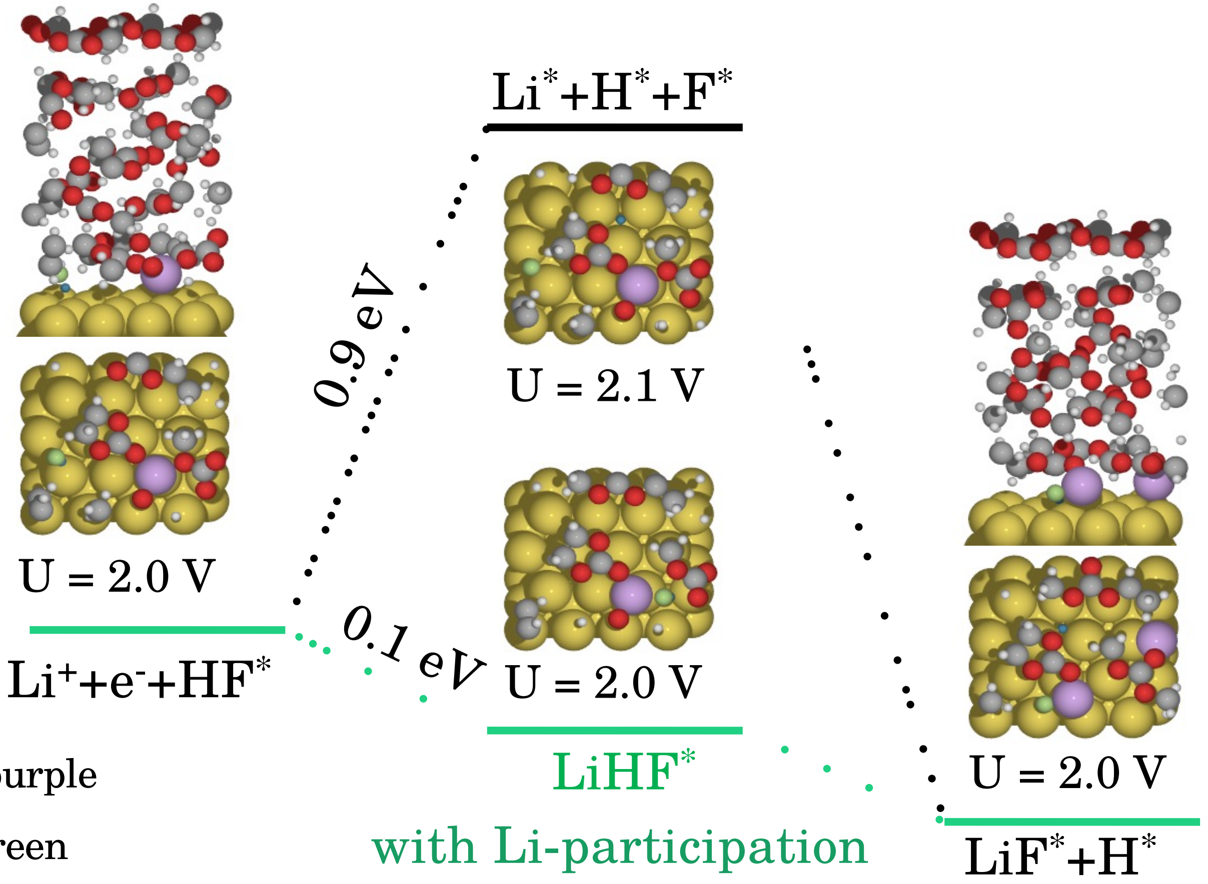

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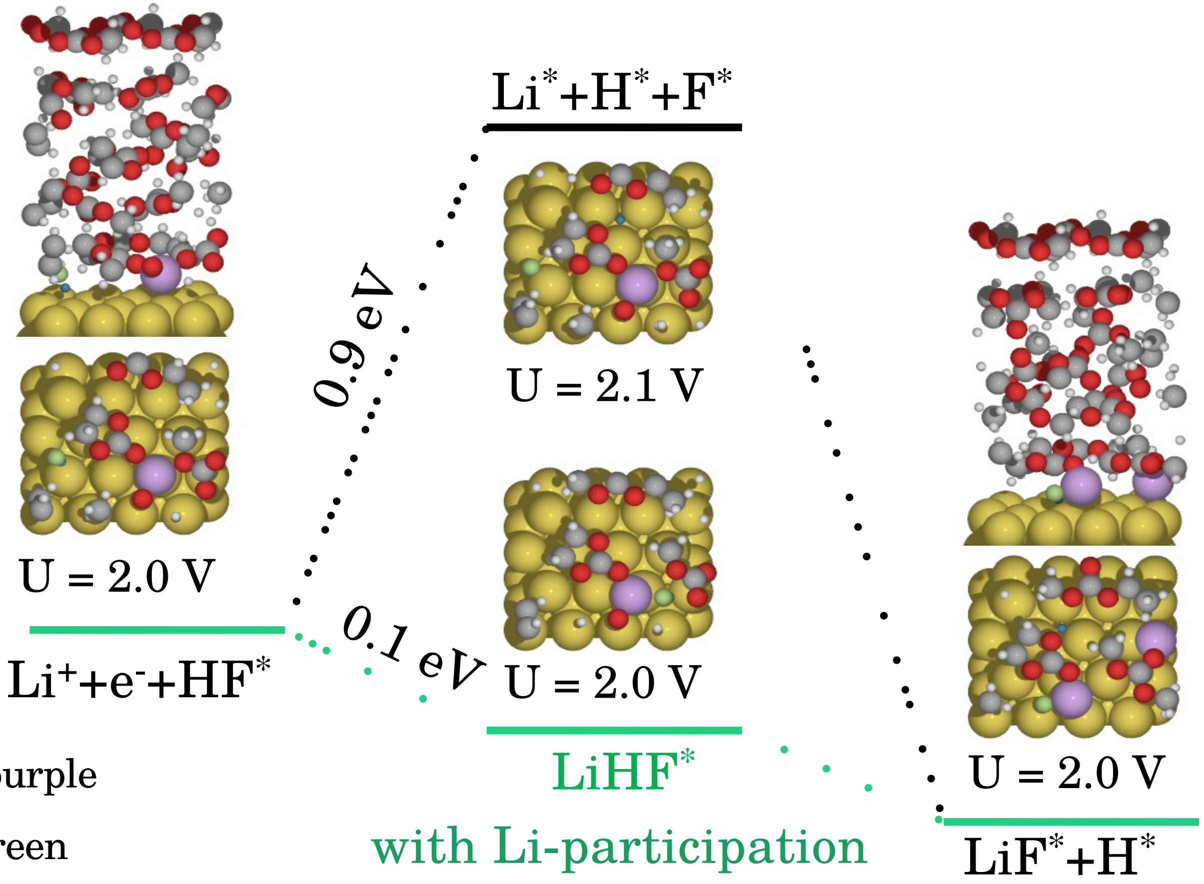
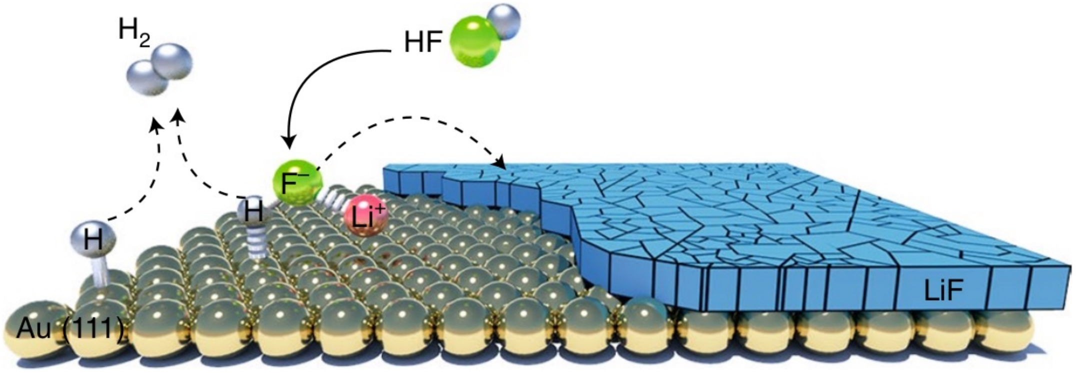


Suggested mechanism



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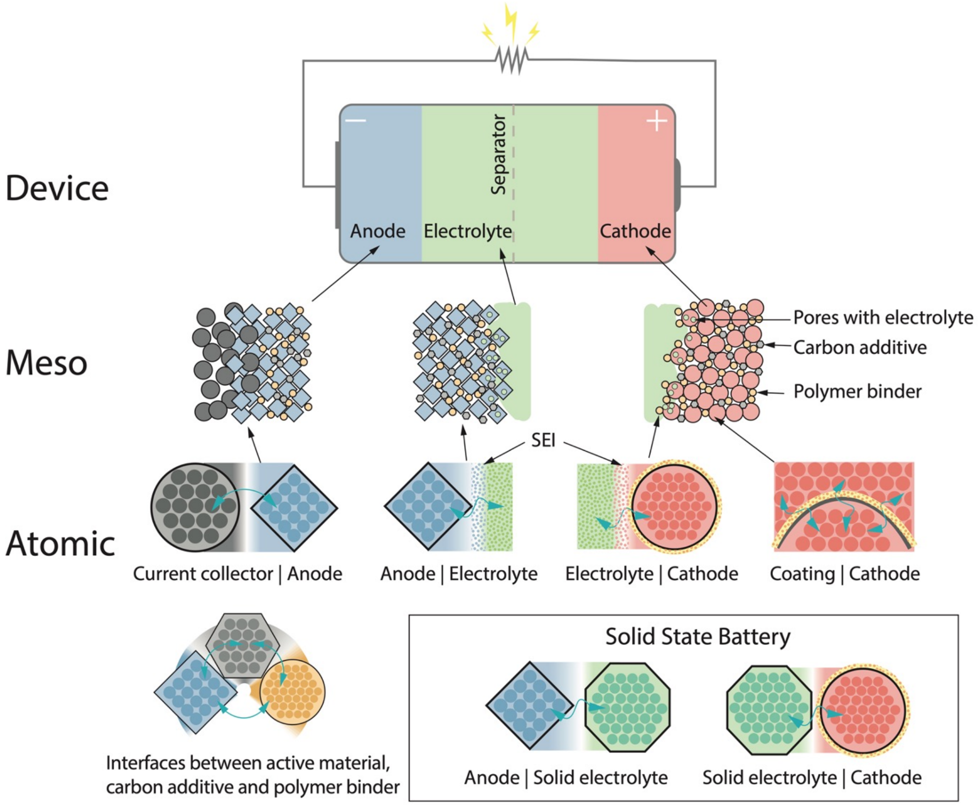
Castelli, Zorko, …, Strmcnik, and Rossmeisl, *Chem. Sci.* **11**, 3914 (2020)

Steps for a Possible Workflow



Inspired by the Atomic Scale Recipes (ASR), Go modular!

1) Workflow for adsorption energies
2) Workflow for MDs
3) Workflow for reaction paths/NEBs

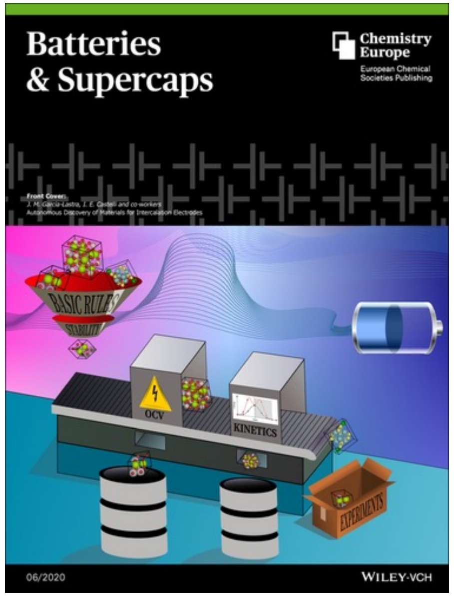
Deng, Kumar, Bölle, Caro, Franco, Castelli, Canepa, Seh, under review (2021)

Conclusions

- Accelerated design and investigation of 1D nanotubes (single-, multi-walls, various prototypes, from stability, to electronic and catalytic properties)
- Autonomous workflow for battery materials (intercalation and solid state electrodes)
- Workflows for interfaces… are we there yet? Let's go modular

Acknowledgements

- **Technical University of Denmark (DK):** Felix T. Bölle, August E. G. Mikkelsen, Kai Zheng, Zhenyun Lan, Nicolai R. Mathiesen, Alexander J. Nielsen, Nestor Chatenet, Andrea Fedrigucci, Theresa Kapunan, Katrine L. Svane, F. N. T. A., Juan Maria Garcia-Lastra, Kristian S. Thygesen, Tejs Vegge
- **University of Copenhagen (DK):** Thomas M. Østergaard, Hao Wan, Jan Rossmeisl
- **Argonne National Laboratory (USA):** Dusan Strmcnik, Nenad Markovic
- **BMW Group (D):** Konstantinos Antonopoulos, Filippo Maglia



Contact: ivca@dtu.dk

Heatmaps of radiuses of Janus nanotubes

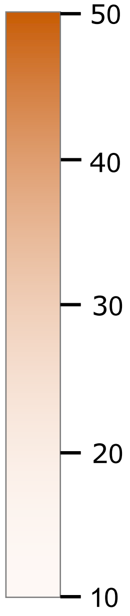
R_min(Å)

Armchair

	SeTe	SSe	STe	S_2	Se_2	Te_2
PbGe	13.81	16.67	10.75	29.23	24.62	22.11
PbSn	23.36	34.25	16.32	57.85	121.89	101.82
SnGe	15.09	16.45	10.62	29.96	26.69	28.36
Pb_2	25.19	25.47	17.02			
Sn_2	24.5	42.85	20.1			
Ge_2	22.65	33.53	17.72			

Zigzag

	SeTe	SSe	STe	S_2	Se_2	Te_2
PbGe	15.37	16.17	11.34	23.77	25.15	25.31
PbSn	25.91	30.76	17.3	67.69	464.28	110.92
SnGe	17.16	18.42	12.19	30.75	32.4	32.38
Pb_2	23.09	41.74	18.62			
Sn_2	24.16	41.6	18.6			
Ge_2	22.12	30.98	17.32			

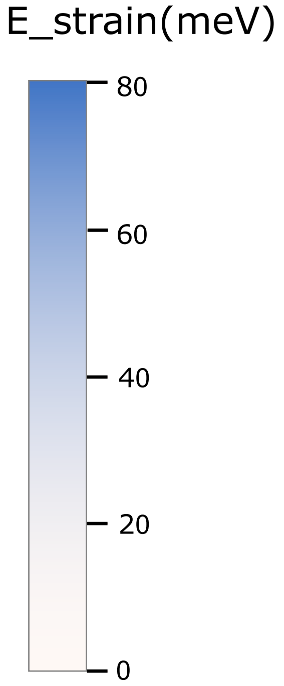


- The GeSPbTe nanotube shows the smallest R_min.

Heatmaps of E_strain of Janus nanotubes

	SeTe	SSe	STe	S_2	Se_2	Te_2
PbGe	-34.01	-18.40	-41.10	-6.16	-11.91	-18.43
PbSn	-15.40	-3.20	-27.40	-2.19	-0.76	-1.00
SnGe	-29.00	-15.00	-37.10	-3.76	-8.74	-8.97
Pb_2	-48.62	-8.33	-57.95			
Sn_2	-37.82	-5.80	-39.83			
Ge_2	-23.25	-10.24	-21.52			

	SeTe	SSe	STe	S_2	Se_2	Te_2
PbGe	-48.40	-39.00	-78.40	-17.06	-16.62	-20.14
PbSn	-17.90	-4.40	-37.00	-2.63	-0.03	-1.01
SnGe	-36.10	-26.80	-63.00	-8.57	-9.18	-11.22
Pb_2	-46.32	-6.35	-61.58			
Sn_2	-35.76	-5.72	-43.67			
Ge_2	-24.09	-10.41	-32.76			



- The GeSPbTe nanotube with the zigzag direction shows the most negative E_strain.