Density-Functional Theory for Practitioners - Lecture 1

Orlando Silveira Júnior, Adolfo Otero Fumega and Ondřej Krejčí,
(Developed by Patrick Rinke and Milica Todorović)

Aalto University
School of Science
Department of Applied Physics

Aalto University
School of Science

Getting to know each other

Go to the white board and write:

- your name
- your country of origin
- a hobby or past-time you enjoy

The course - Basic information

Dates: 5.9 - 1.12.2019
Credits: 5 ECR

MyCourses page:

https://mycourses.aalto.fi/course/view.php?id=36086

Time line

Period 1 (5.9. - 14.10.)

Period 2 (24.10. - 1.12.)

Theory lectures

Mondays

Practical hands-on classes

Thursdays

Project work

Check point

27.10.

Check point

10.11.

Check point

1.12.

Hands-on classes & check points:
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Content

Must know	Should know	Nice to know
Basic principles of computational materials modelling	Relation between certain materials properties and different modelling approaches	Pros and cons of different modelling approaches
Basic principles of density-functional theory (DFT)	The exchange-correlation functional	Strengths and limitations of DFT

Content

Must know	Should know	Nice to know
How to use DFT in computational materials modelling	• Equilibrium structures of materials (e.g., molecules, solids, surfaces) • Elastic properties of materials • Thermodynamics (phase diagrams)	• Vibrations, phonons and vibrational spectroscopy • Band structures and photo-electron spectroscopy • Dielectric function and optical spectra
Basic familiarity with the DFT software package FHI-aims	FHI-aims and its features	Familiarity with Linux

Learning outcomes

After completion of the course you

- Have developed an understanding of DFT-based materials modelling.
- Are familiar with the FHI-aims DFT software package.
- Can solve simple physics, chemistry and material science problems with DFT.
- Can follow a presentation (e.g. conference or seminar) on DFT results.
- Can plan, execute, document and present a small research project.
- Can give peer feedback.

Time line

Period 1 (5.9. - 14.10.)

Period 2 (24.10. - 2.12.)

02. 2013

Virtual Winter School on Computational Chemistry

NEXT edition February 2023

More info at:

https://winterschool.cc/home/news/winterschool

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27.10.

10.11.

1.12.

Project proposal deadline 24.10
Project report deadline 5.12

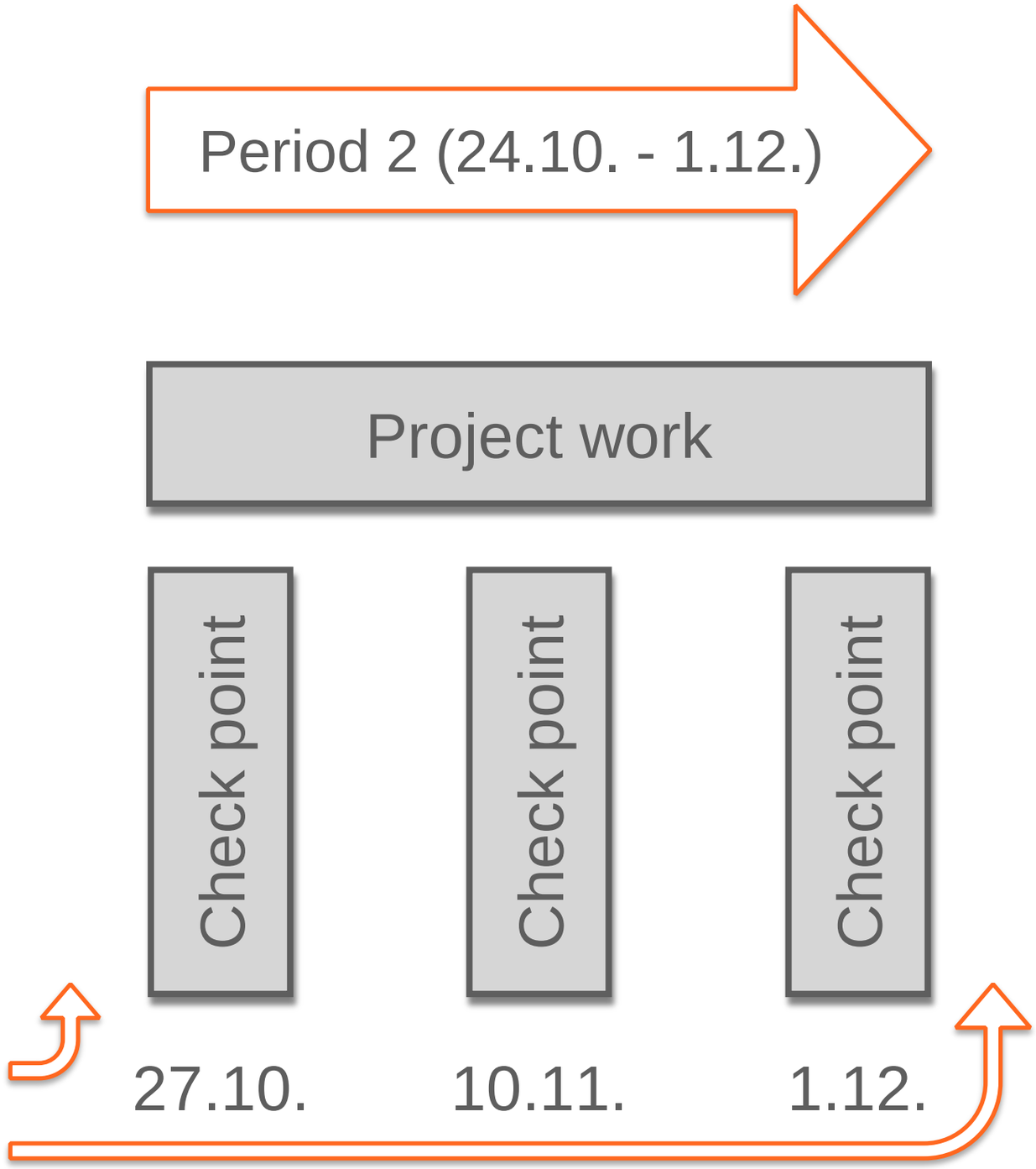
Project work

Project:

Propose and solve an original problem with DFT.

The problem can be:
- from your own research.
- something you are interested in.
- something you discover in this course and would like to pursue further.

Must be doable in 6 weeks!



Project timeline

24.10. (end of week 7):	Submit project plan
27.10. contact session:	Project presentations
10.11. contact session:	Progress report presentations
01.12. contact session:	Final results presentations
05.12. dead line	Submit final report

Assessment

assessed by teacher

Submit project plan

feedback from teachers

Project presentations

peer feedback

Progress report presentations

peer/teachers feedback

Final results presentations

assessed by teacher

Submit final report

Course requirements

The 5 ECR credits are awarded if you:

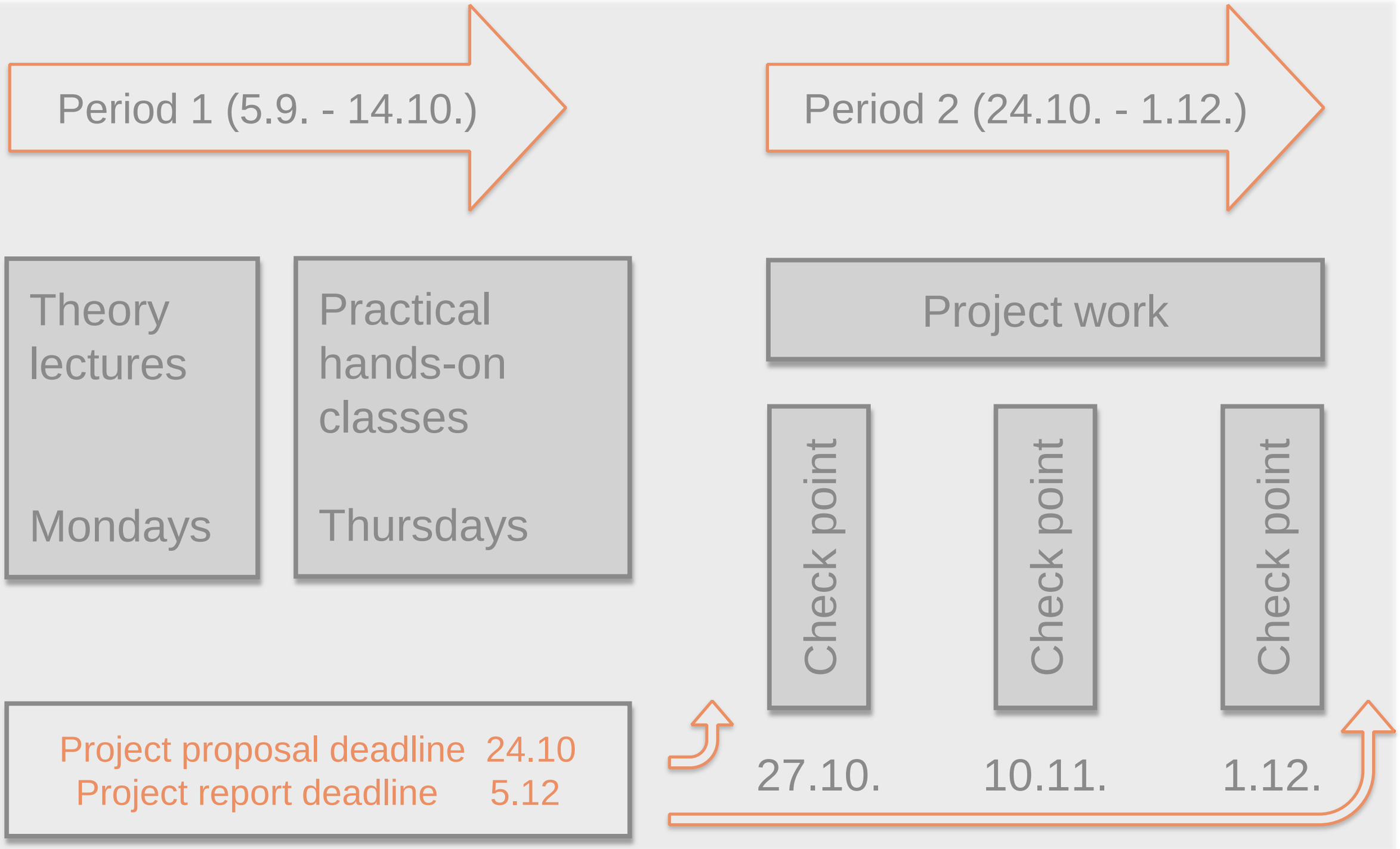
- attend at least 5 out of the 6 practical sessions*
- submit the project proposal
- attend at least 2 out of the 3 project check points*
- submit 3 project presentations
- complete the project
- submit the final project report

*if not fulfilled, additional assessment possible

Work load

Activity	Time per week	Frequency	Total
Period 1			
Contact session	2h	6	12h
Reading for contact session	1h	6	6h
Hands-on session in computer lab	4h	6	24h
Time to think and reflect	3h	6	18h
Planning project work	3h	1	3h
Writing project plan	4h	1	4h
			67h
Period 2 – Project Work			
Contact Session	4h	3	12h
Preparing project plan and progress presentation	3h	3	9h
Project work	7h per week	6	42h
Writing final report	4h	1	4h
			67h
			134h

Questions ?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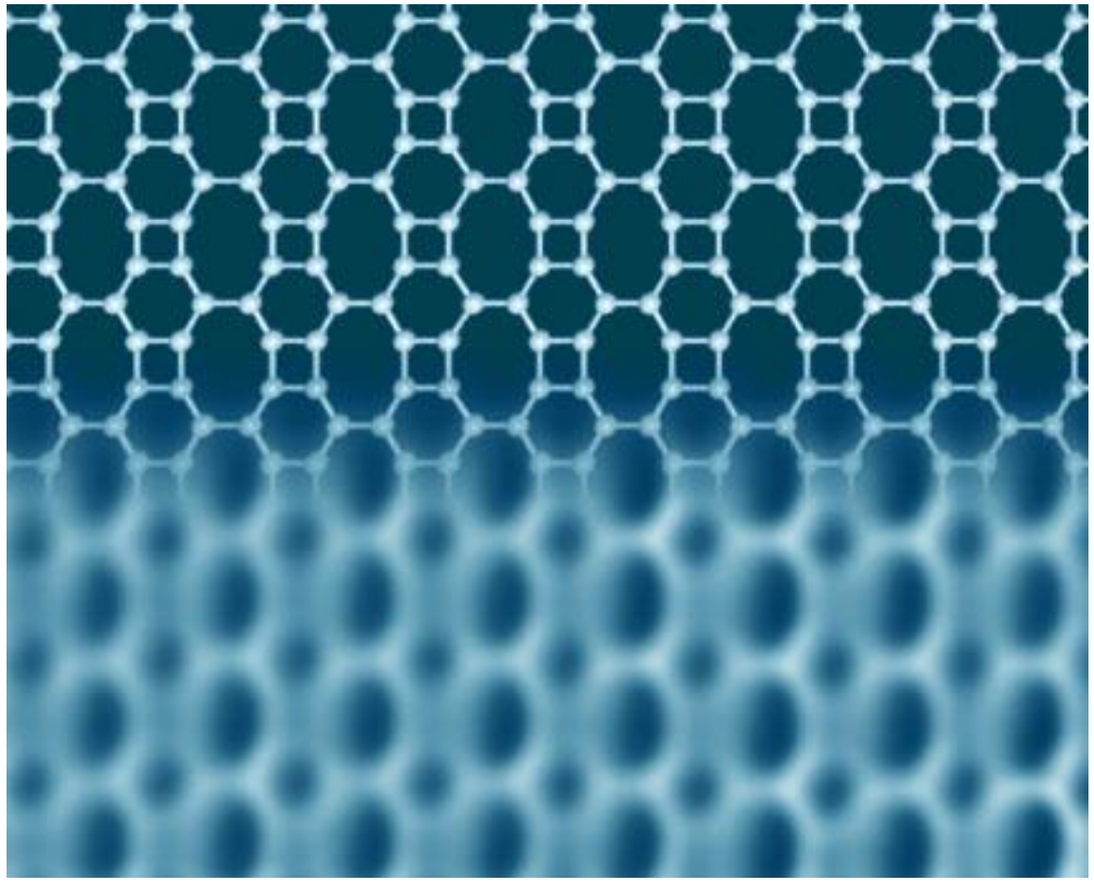
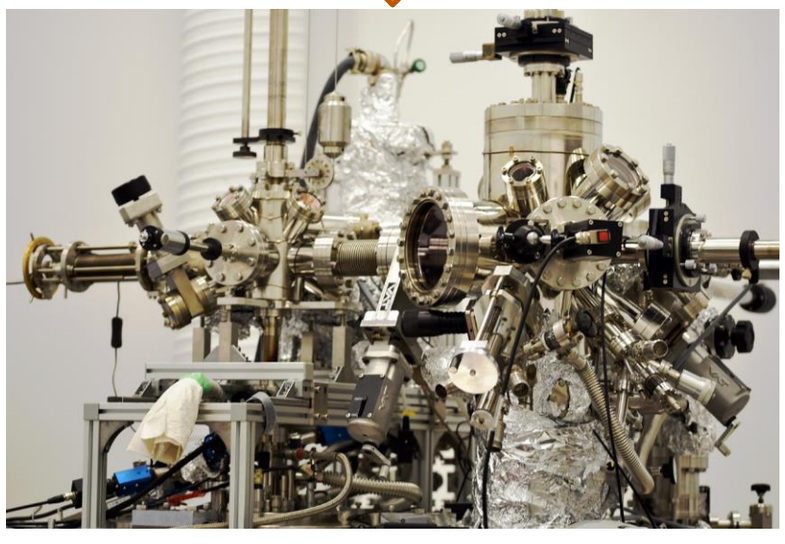
Materials Modelling





This class - content

Must know	Should know	Nice to know
Basic principles of computational materials modelling	Relation between certain materials properties and different modelling approaches	Pros and cons of different modelling approaches
The three “principles” of density-functional theory (DFT)	Variational principle	Quantities that can be calculated with DFT

This class - learning outcomes

After the class today you

- have a first impression of materials modelling as a context for DFT.

- know the three “principles of DFT”.

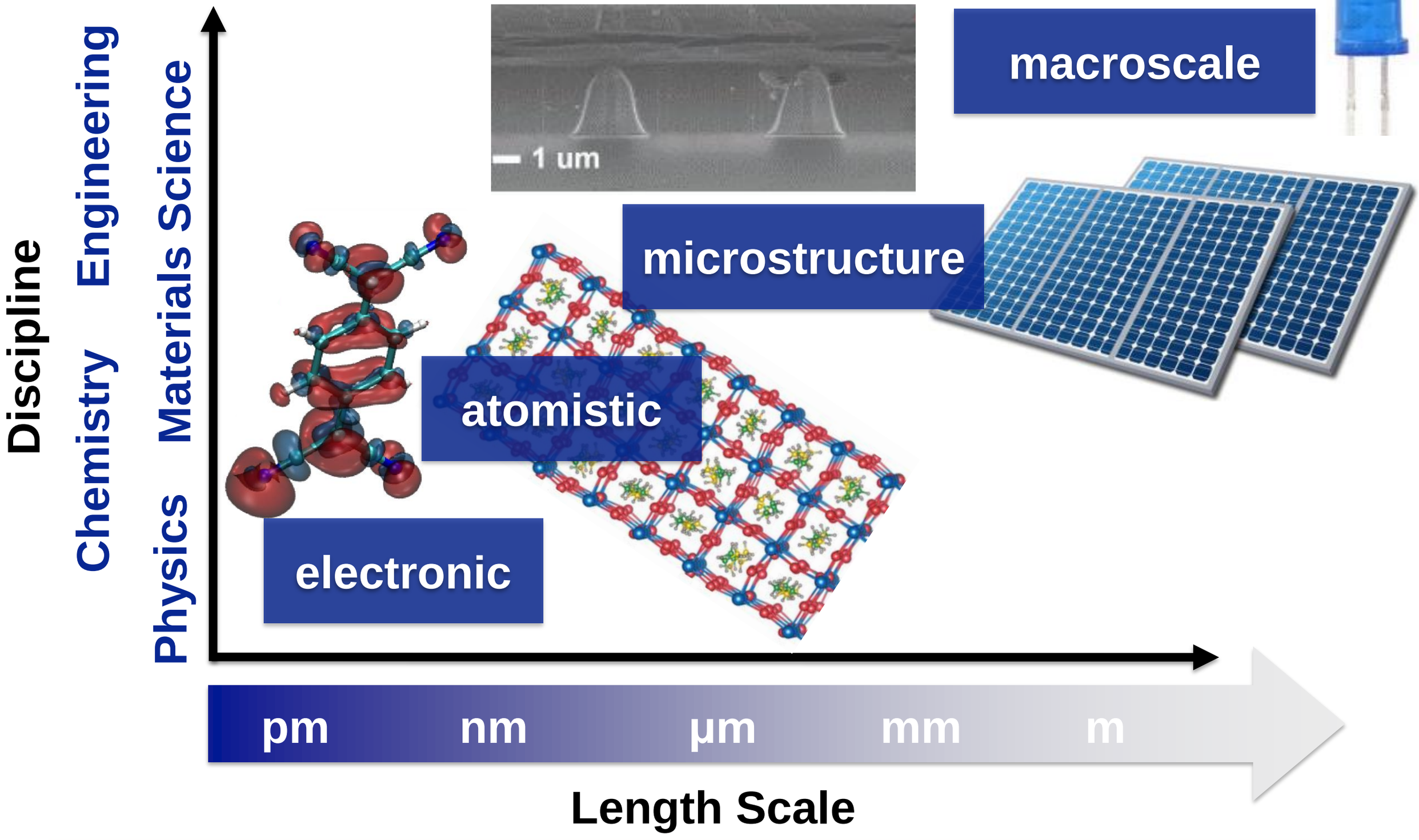
Materials modeling - a discussion

Discuss in your group:

What is materials modelling?

- What can be modelled? (What is modelled in science/industry?)
- What materials modelling approaches do you already know?
- What are the strength and weaknesses of modelling, e.g. compared to experimentally characterising a material?

Materials modelling - Length scales



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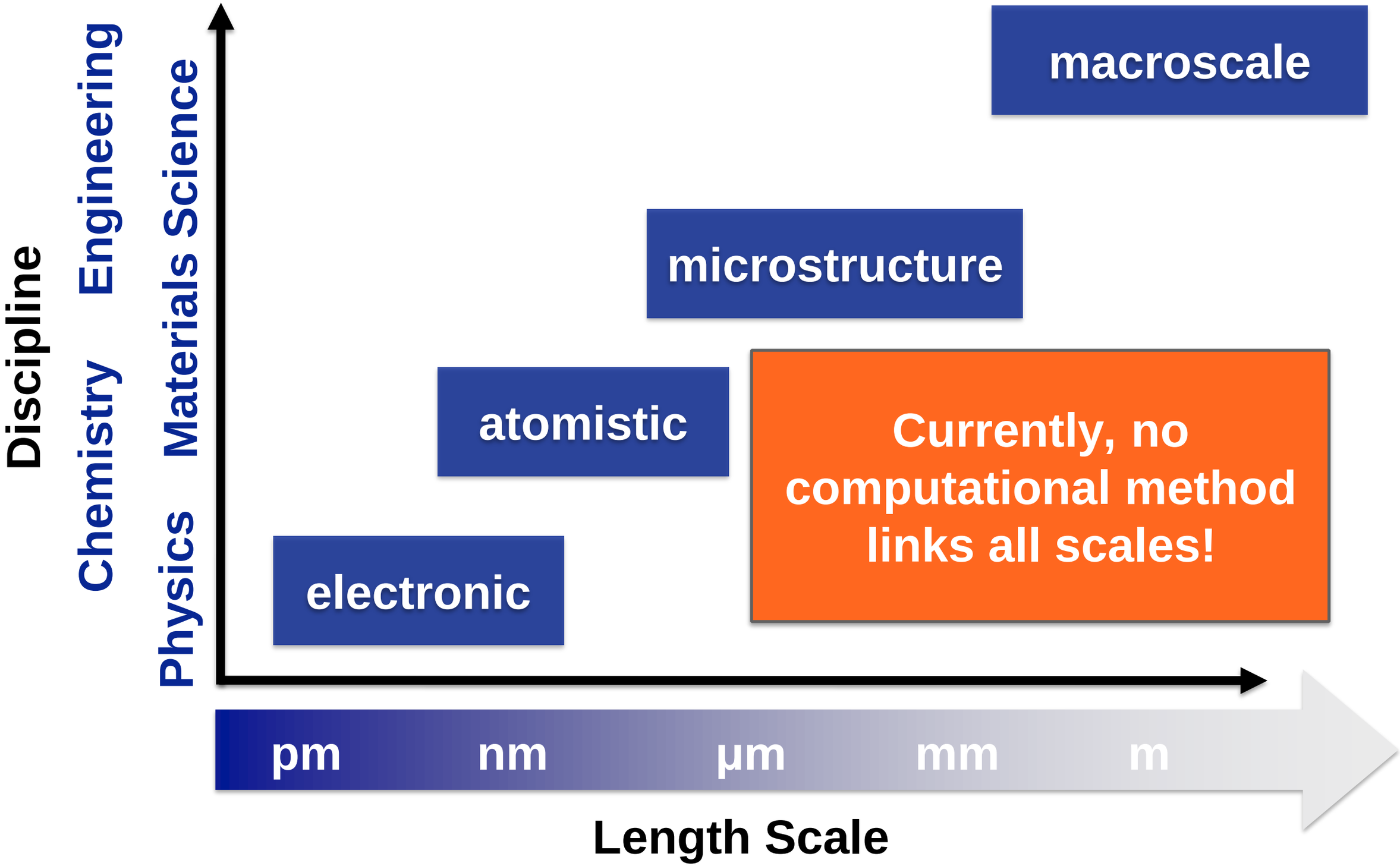
Electron micrograph courtesy of Sami Suihkonen @ Aalto

Multi-scale modelling of materials



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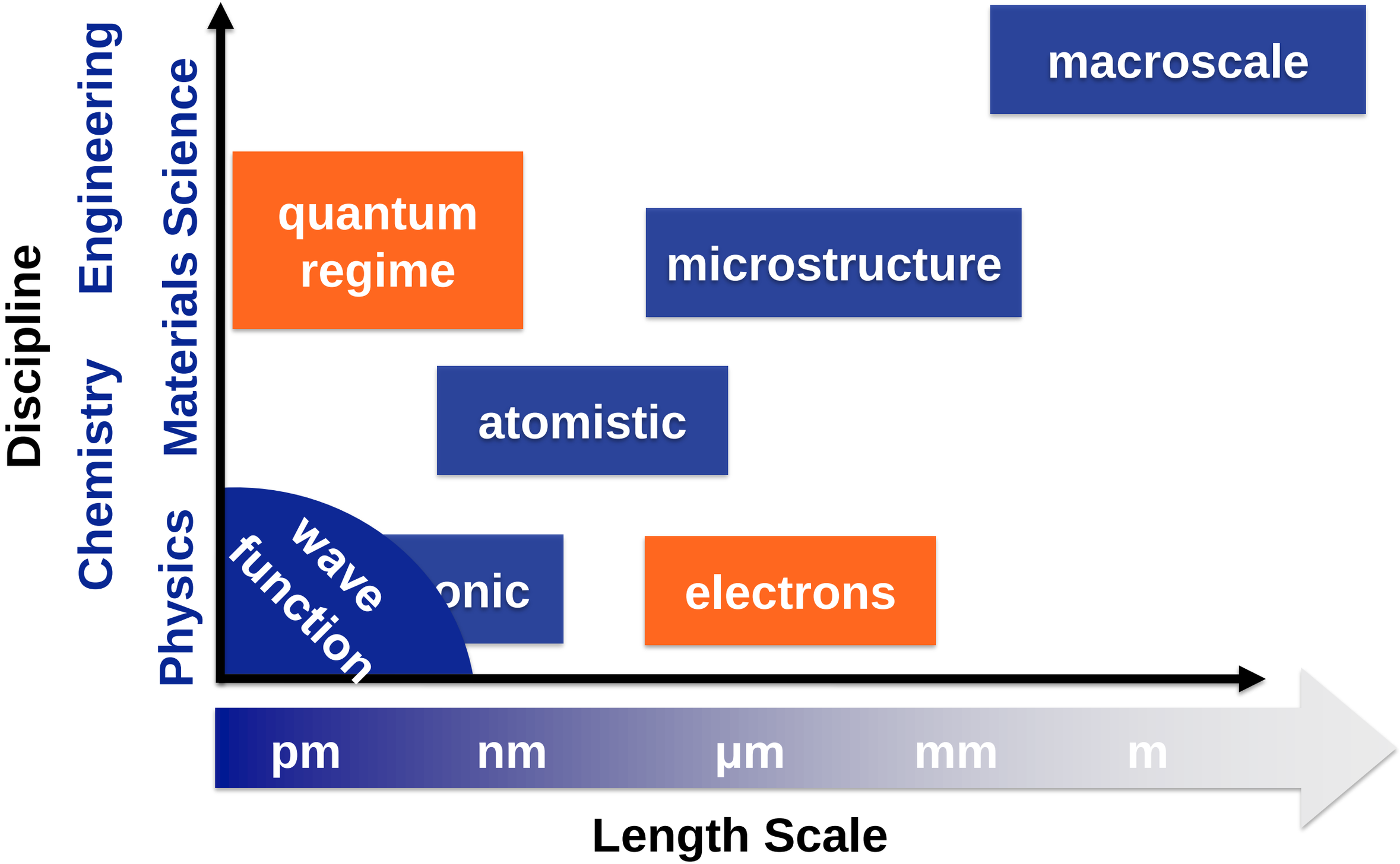
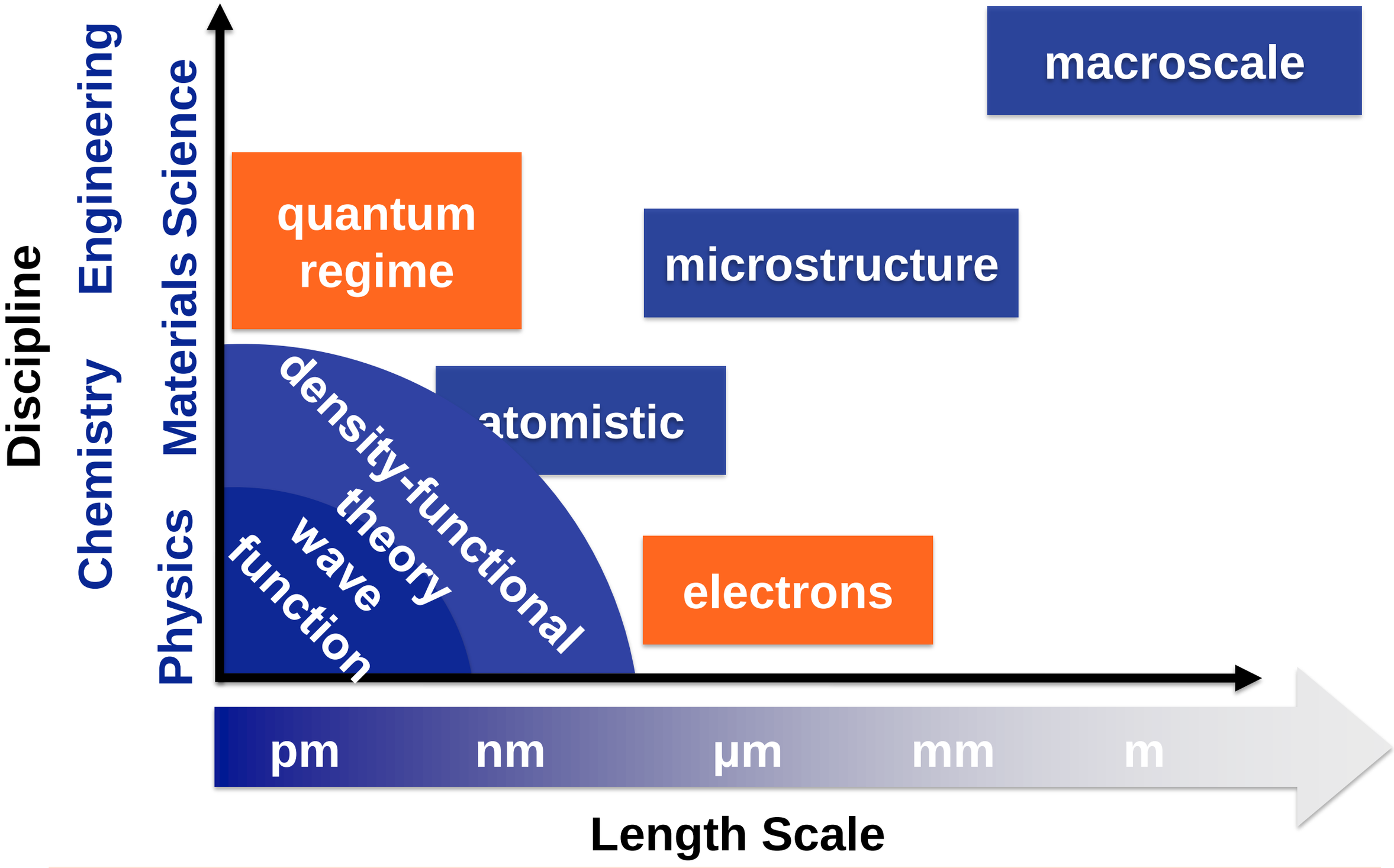


Multi-scale modelling of materials



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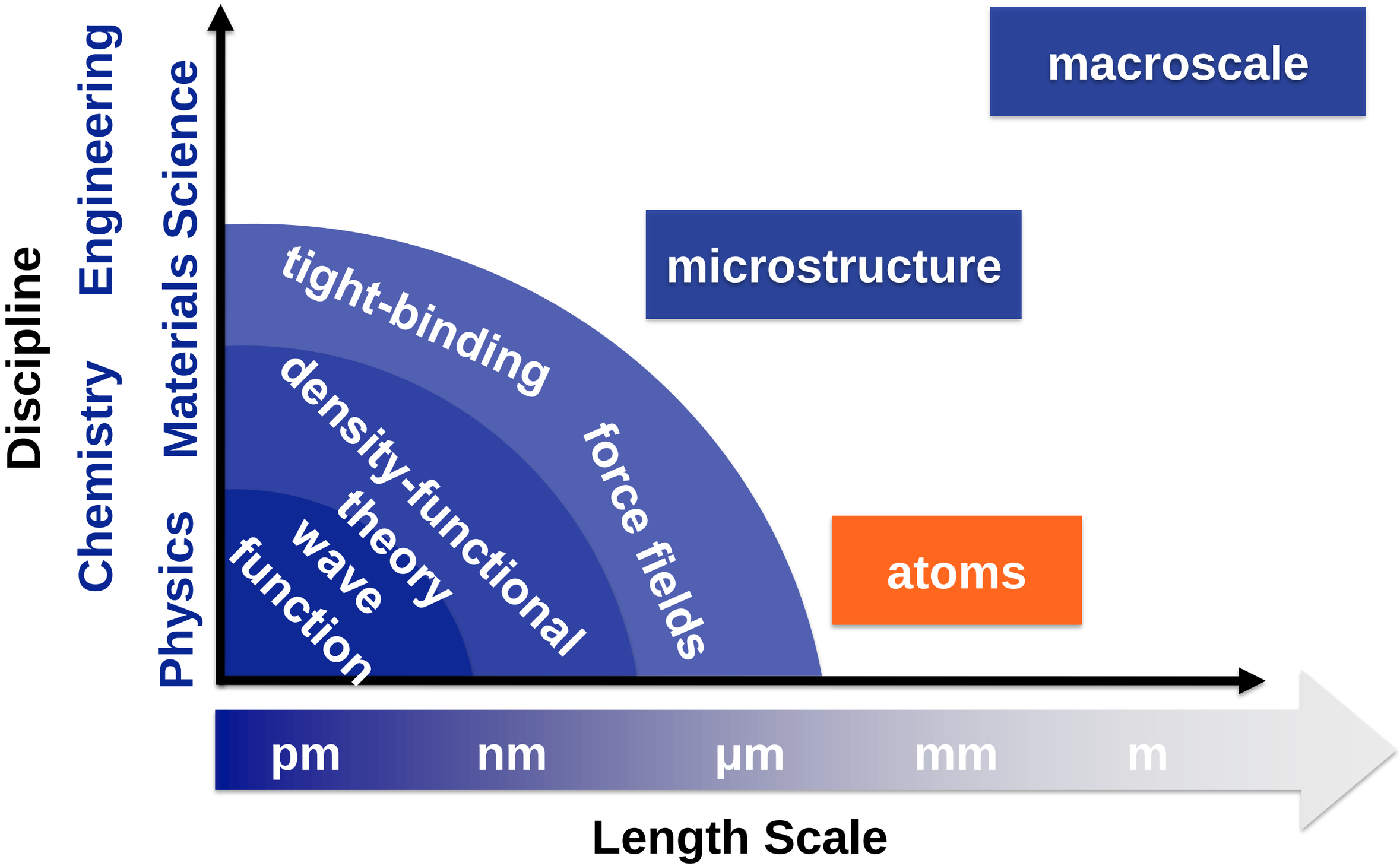

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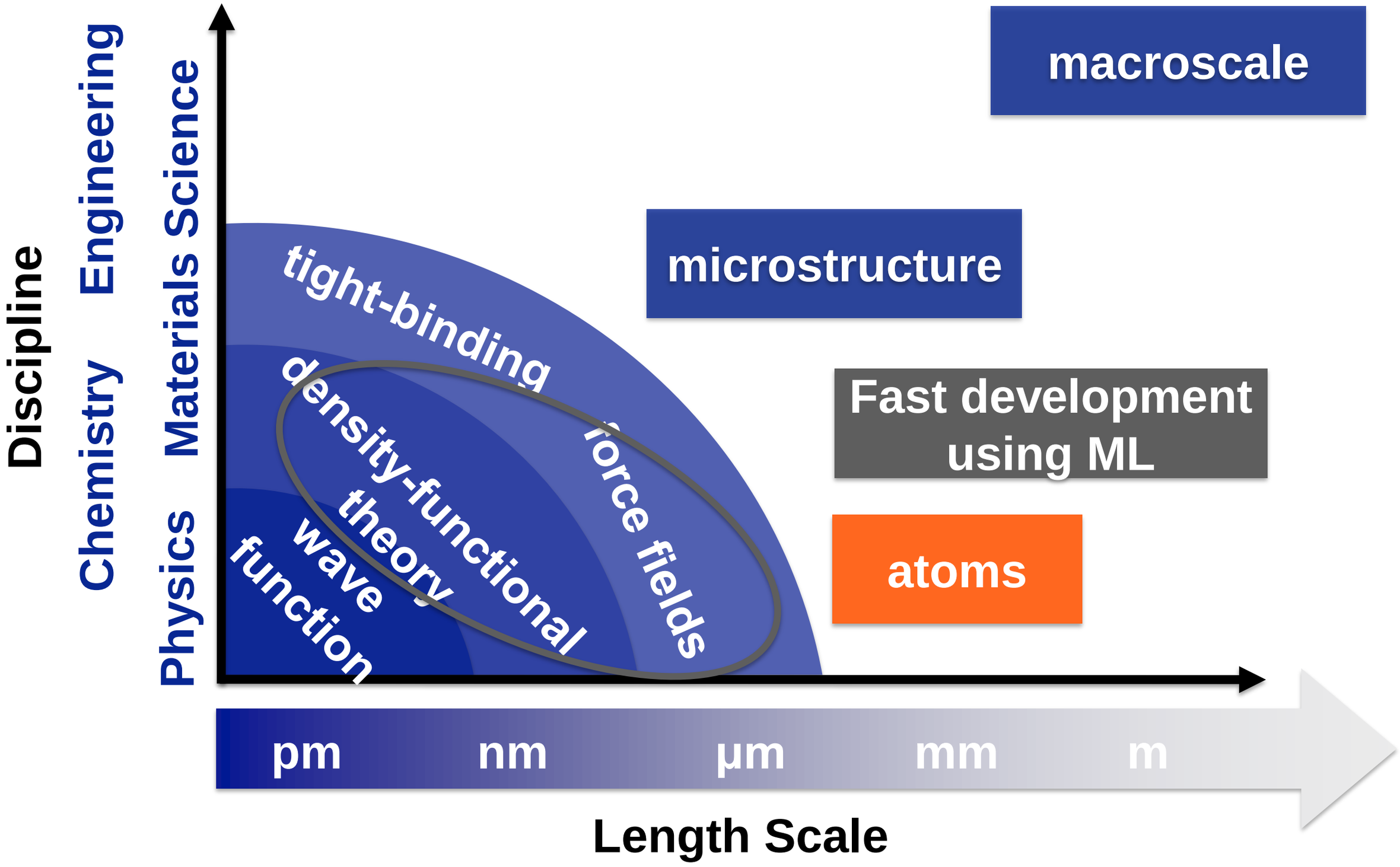
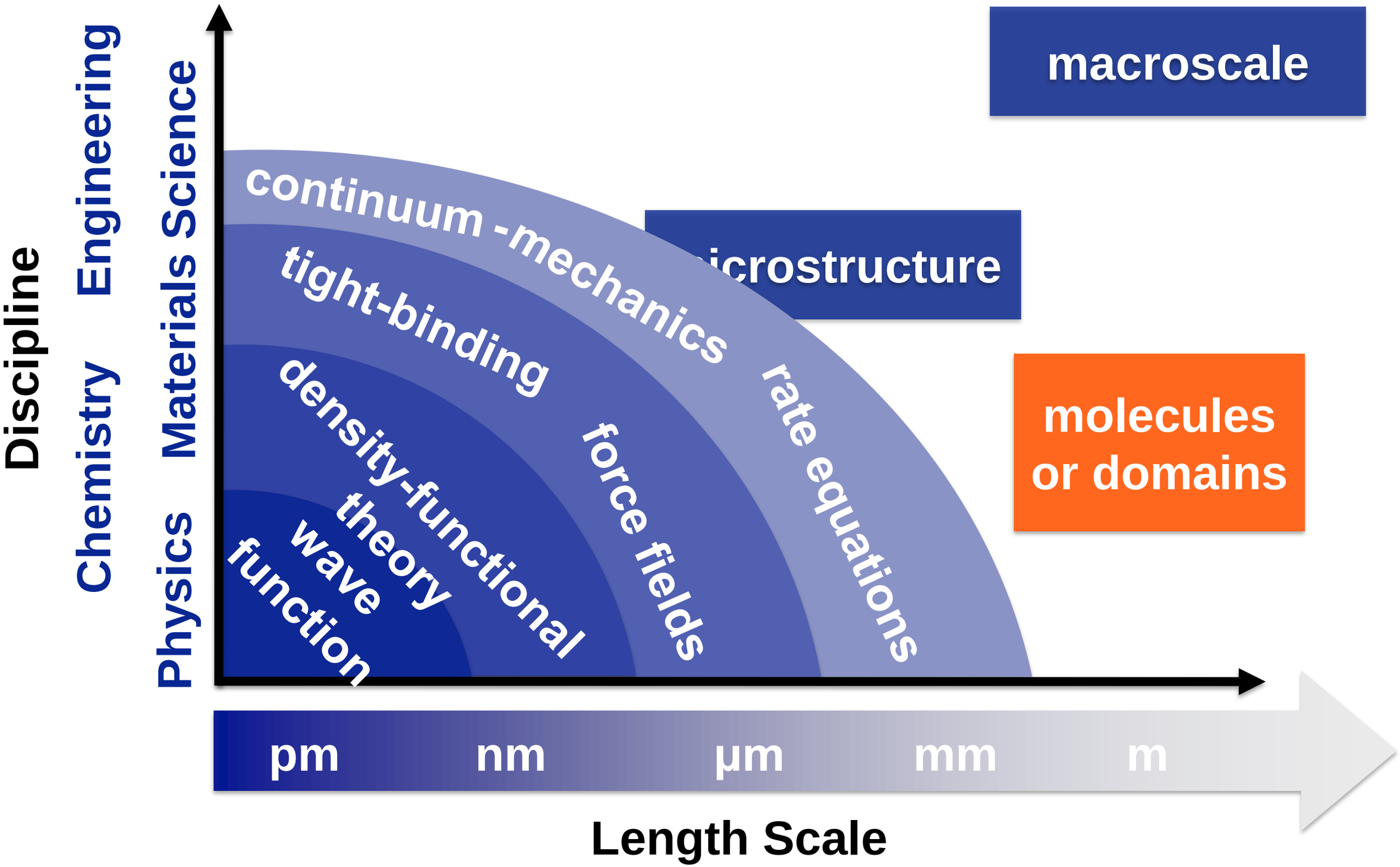


Multi-scale modelling of materials



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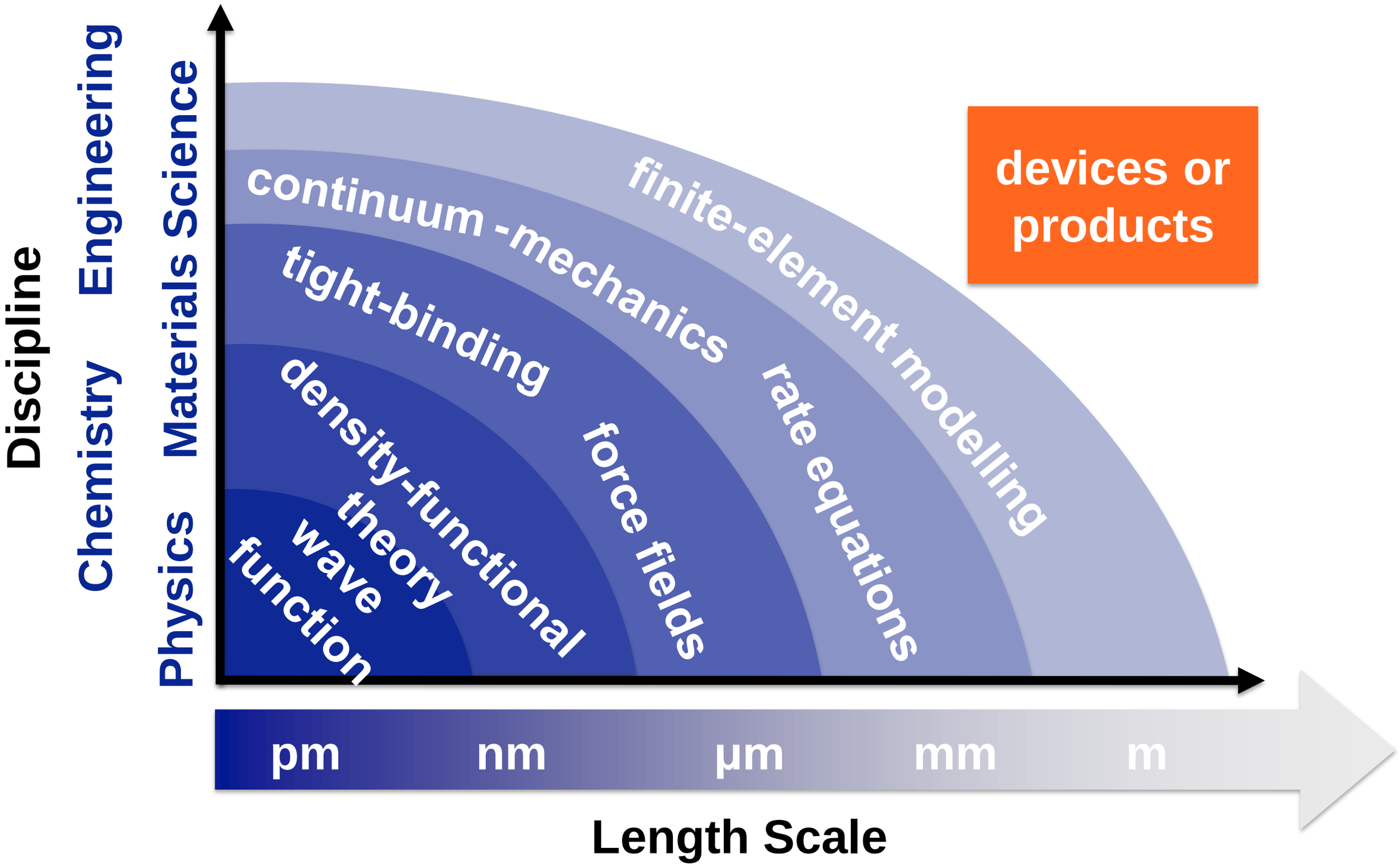
Multi-scale modelling of materials



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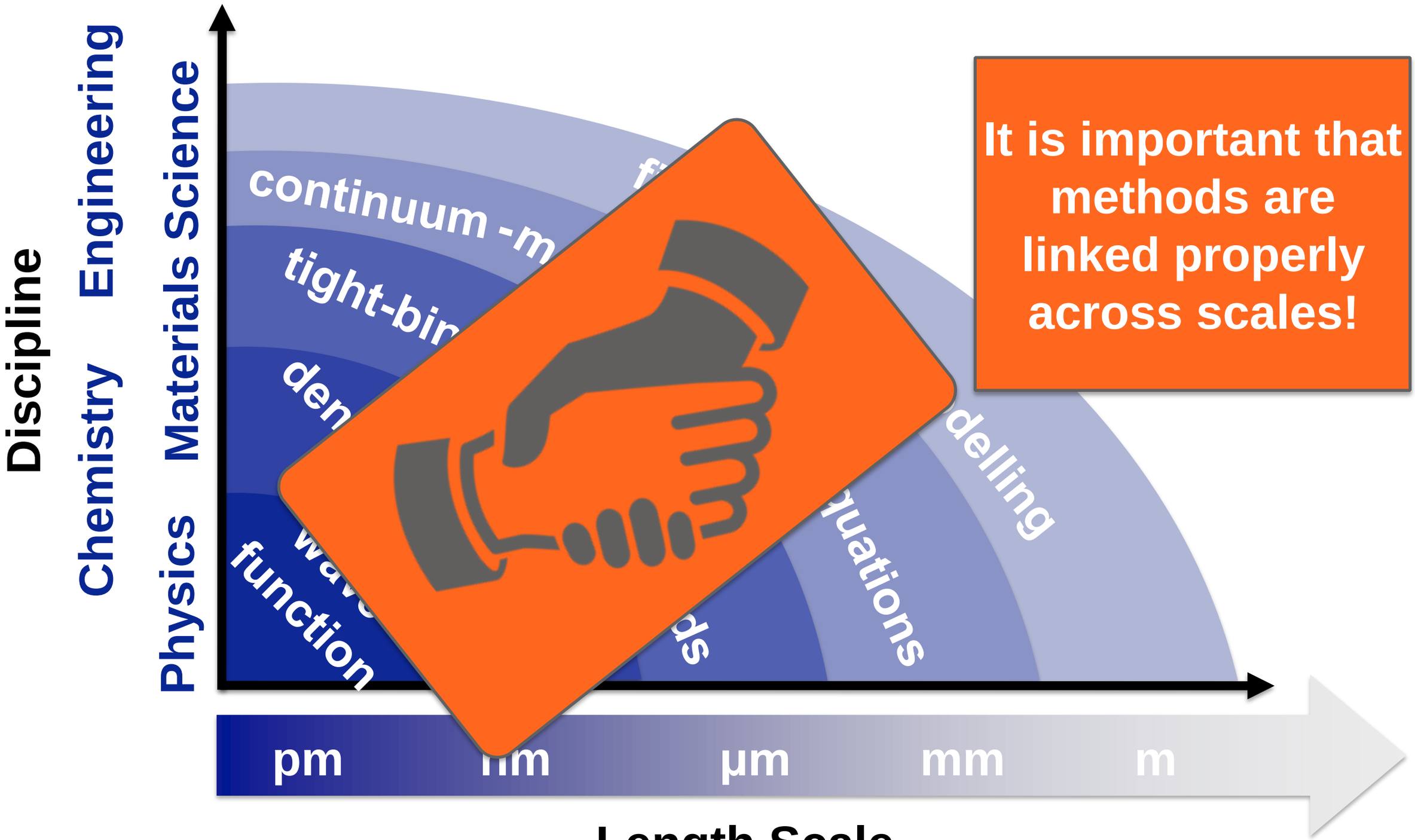
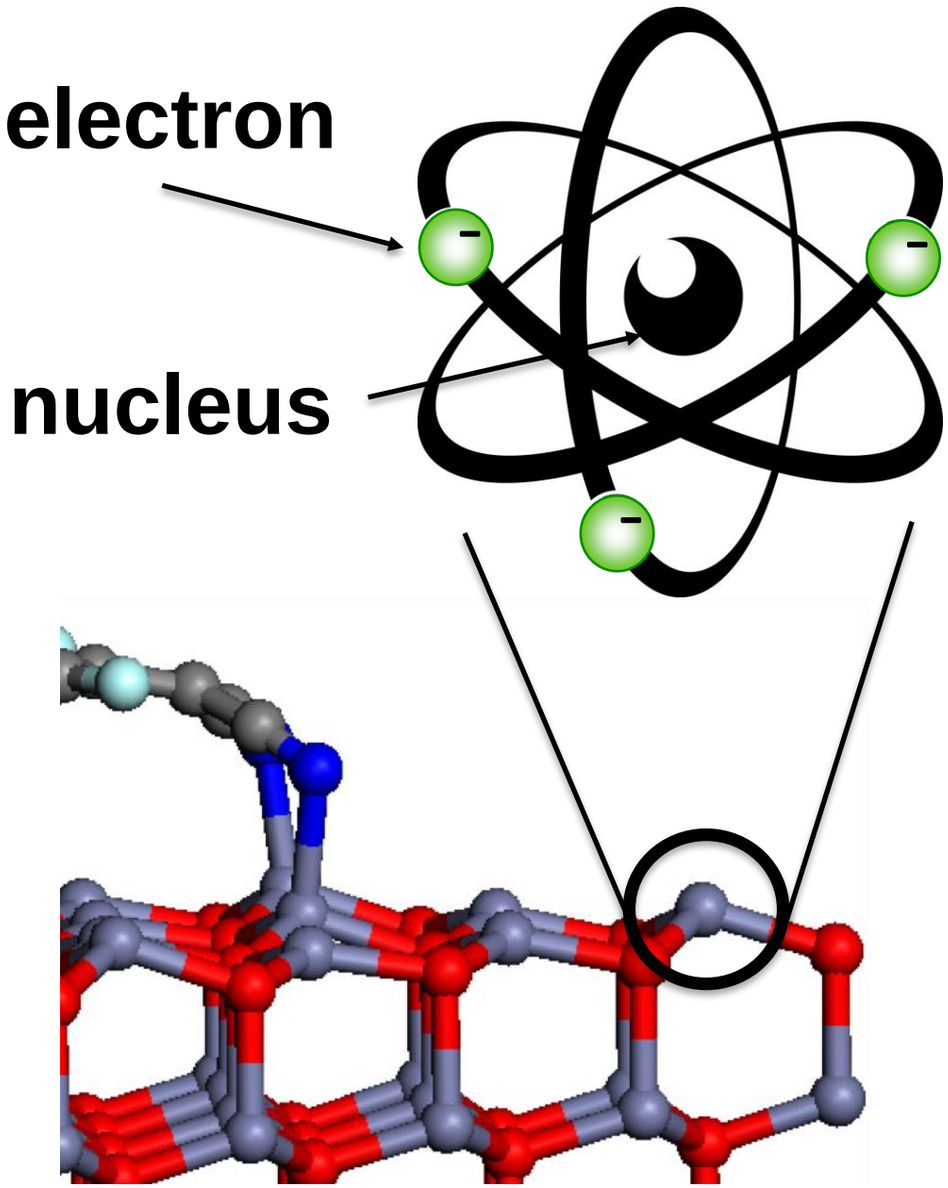


It is important that methods are linked properly across scales!

Non-relativistic quantum mechanics



Quantum mechanics:

- **Schrödinger equation**

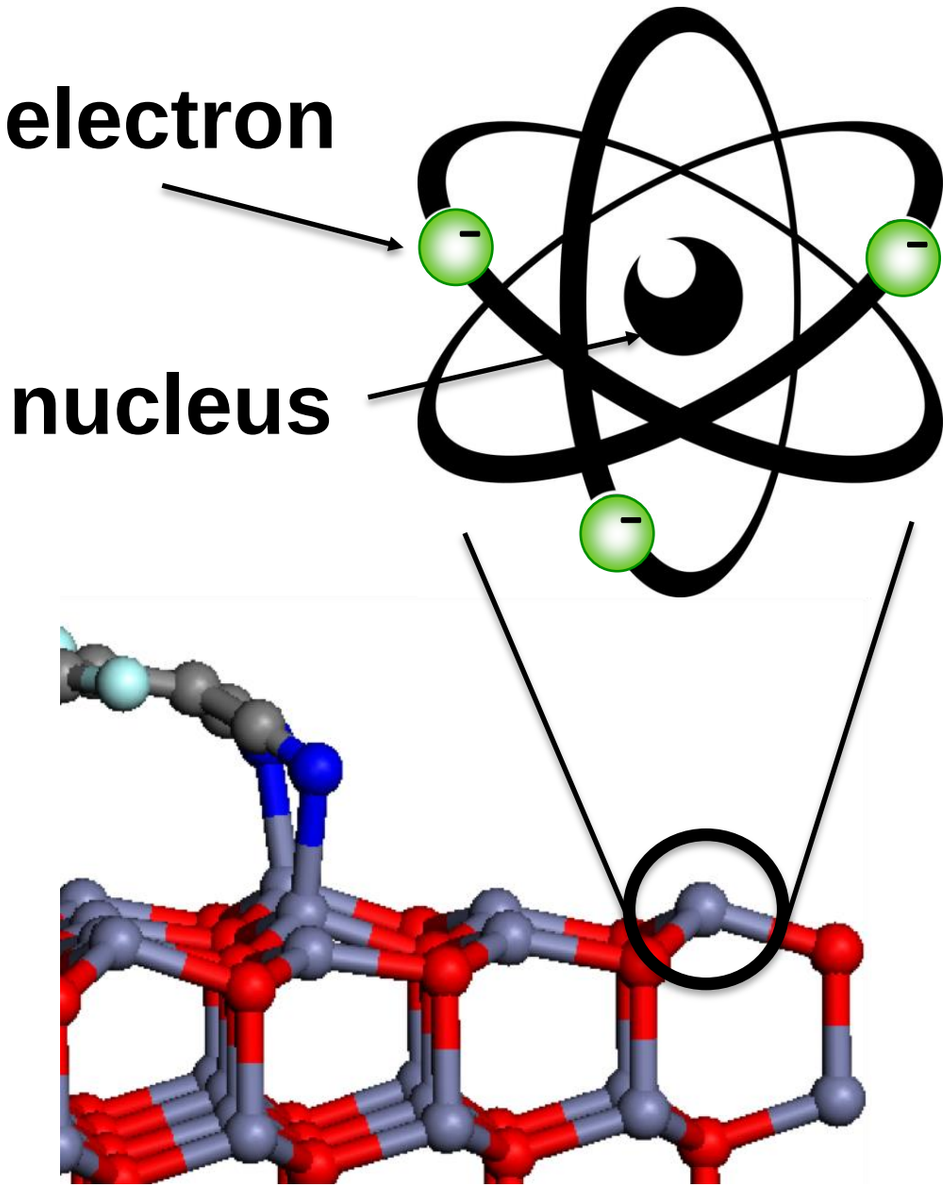
$$H\Psi = E\Psi$$

Hamilton operator
(brings in system specific information**)**

wave function

energy

Non-relativistic quantum mechanics



Quantum mechanics:

- **Schrödinger equation**

$$H\Psi = E\Psi$$

H(...)

Ψ(...)

The full Hamiltonian

$$H(\bullet\bullet\bullet \ \ldots \ \ominus\ominus\ominus \ldots)$$

$$\mathcal{H} = \overbrace{-\sum_{I=1}^{N_n} \frac{\nabla^2_{\mathbf{R}_I}}{2M_I}}^{T^n} + \overbrace{\sum_{I=1}^{N_n}\sum_{J>I}^{N_n} \frac{Z_I Z_J}{|\mathbf{R}_I - \mathbf{R}_J|}}^{V^{nn}}$$

$$\underbrace{-\sum_{i=1}^{N_e} \frac{\nabla^2_{\mathbf{r}_i}}{2}}_{T^e} + \underbrace{\sum_{i=1}^{N_e}\sum_{j>i}^{N_e} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}}_{V^{ee}} + \underbrace{\sum_{i=1}^{N_e}\sum_{J=1}^{N_n} \frac{-Z_J}{|\mathbf{r}_i - \mathbf{R}_J|}}_{V^{ne}}$$

Dirac's challenge (1929)

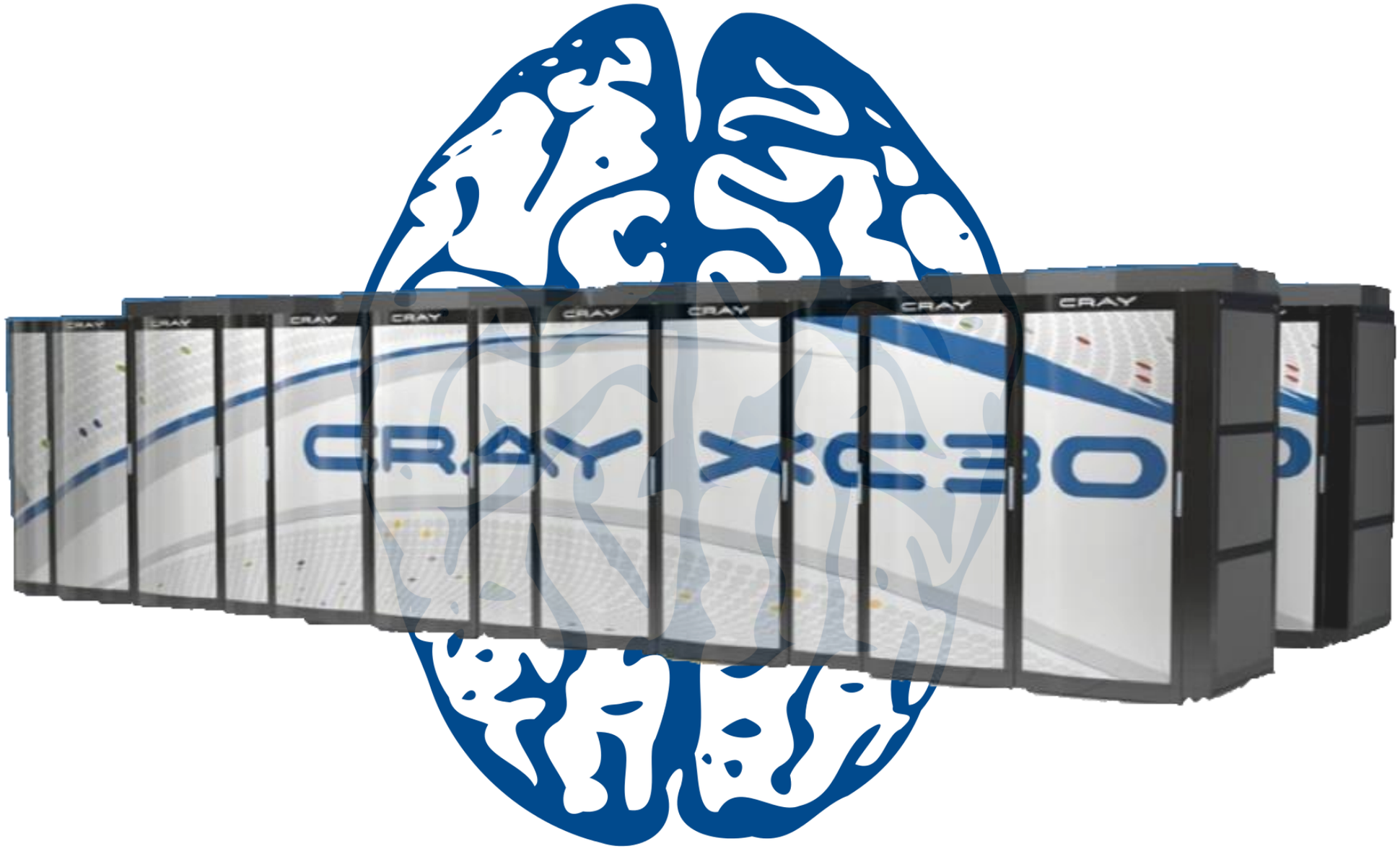
The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.

Paul Dirac

It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.

Proceedings of the Royal Society of London.
Series A, Vol. 123, No. 792 (6 April 1929)

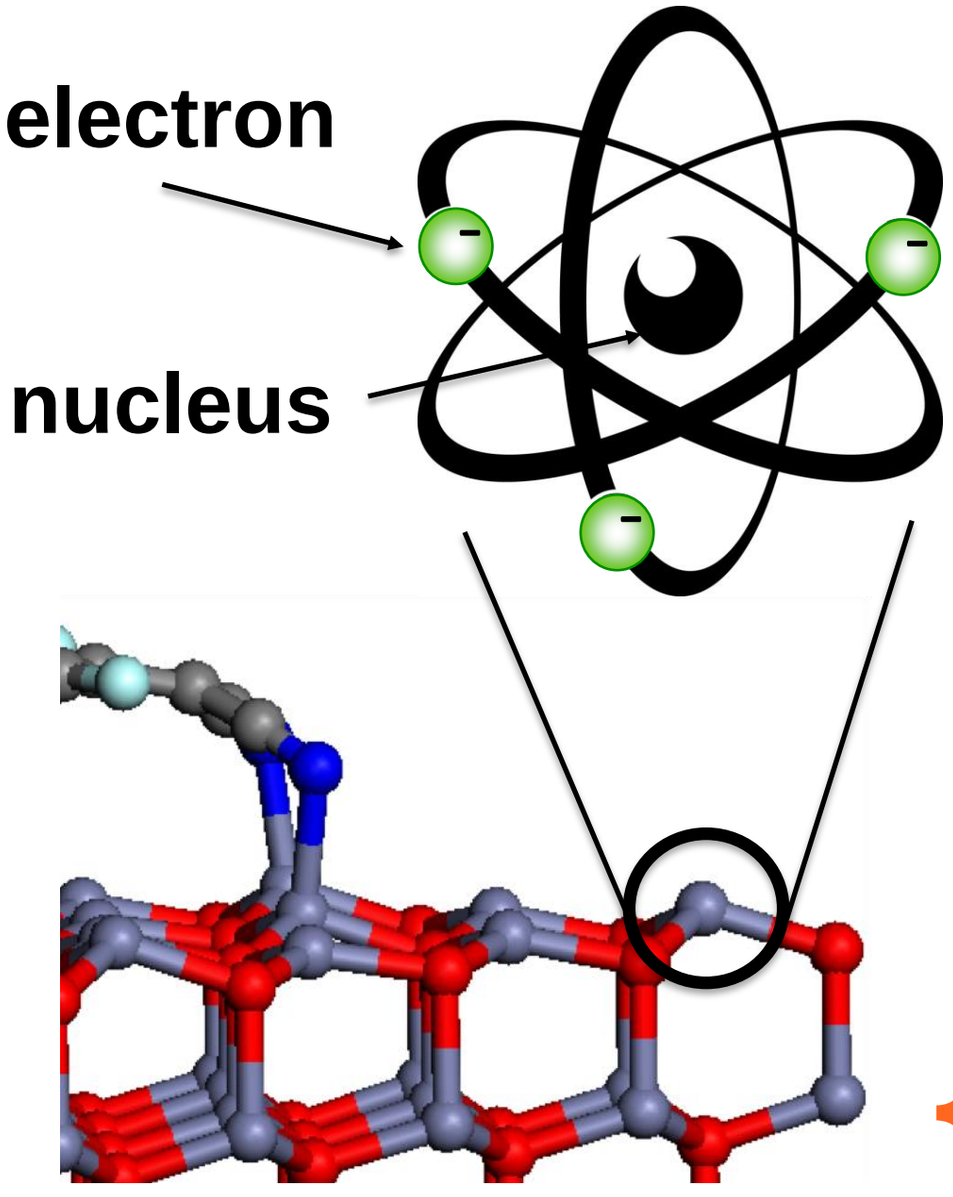
What Dirac didn’t know…



What Dirac didn’t know…

New concepts!

Non-relativistic quantum mechanics

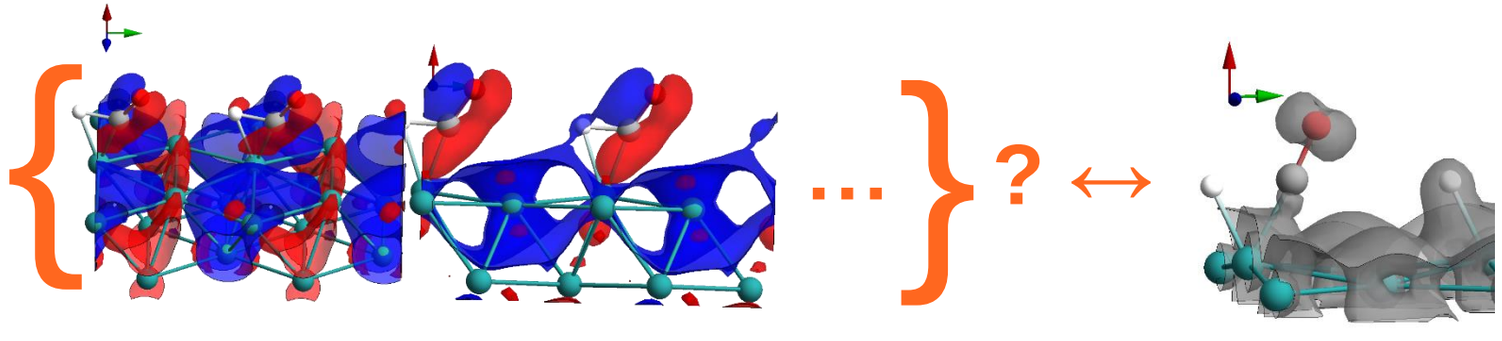


Quantum mechanics:

- **Schrödinger equation**

$$H\Psi = E\Psi$$

$$\Psi(\bullet\bullet\bullet \ldots \ominus\ominus\ominus \ldots)$$



DFT - Hohenberg-Kohn theorems

Theorem 1:

The ground state density $n_0(r)$ uniquely determines the potential up to an arbitrary constant.

$$v_{\text{ext}}(\mathbf{r}) \Leftrightarrow n_0(\mathbf{r})$$

$$\underbrace{-\sum_{i=1}^{N_e}\frac{\nabla_{\mathbf{r}_i}^2}{2}}_{T^e} + \underbrace{\sum_{i=1}^{N_e}\sum_{j>i}^{N_e}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}}_{V^{ee}} + \underbrace{\sum_{i=1}^{N_e}\sum_{J=1}^{N_n}\frac{-Z_J}{|\mathbf{r}_i-\mathbf{R}_J|}}_{V^{ne}}$$

Walter Kohn

Pierre Hohenberg

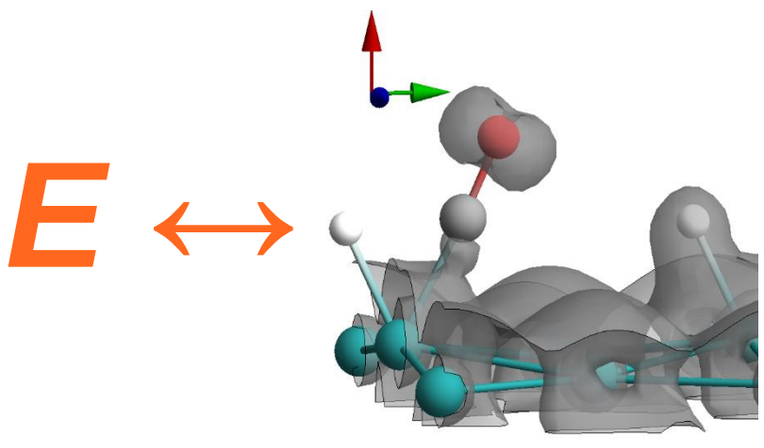
P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964)

DFT - Hohenberg-Kohn theorems

Theorem 2:

A universal functional for the energy *E[n]* in terms of the density *n(r)* can be defined, valid for any external potential $v_{ext}(r)$.

For any given $v_{ext}(r)$, the exact ground state energy of the system is the global minimum of this functional and the density that minimizes the functional is the exact ground state density.



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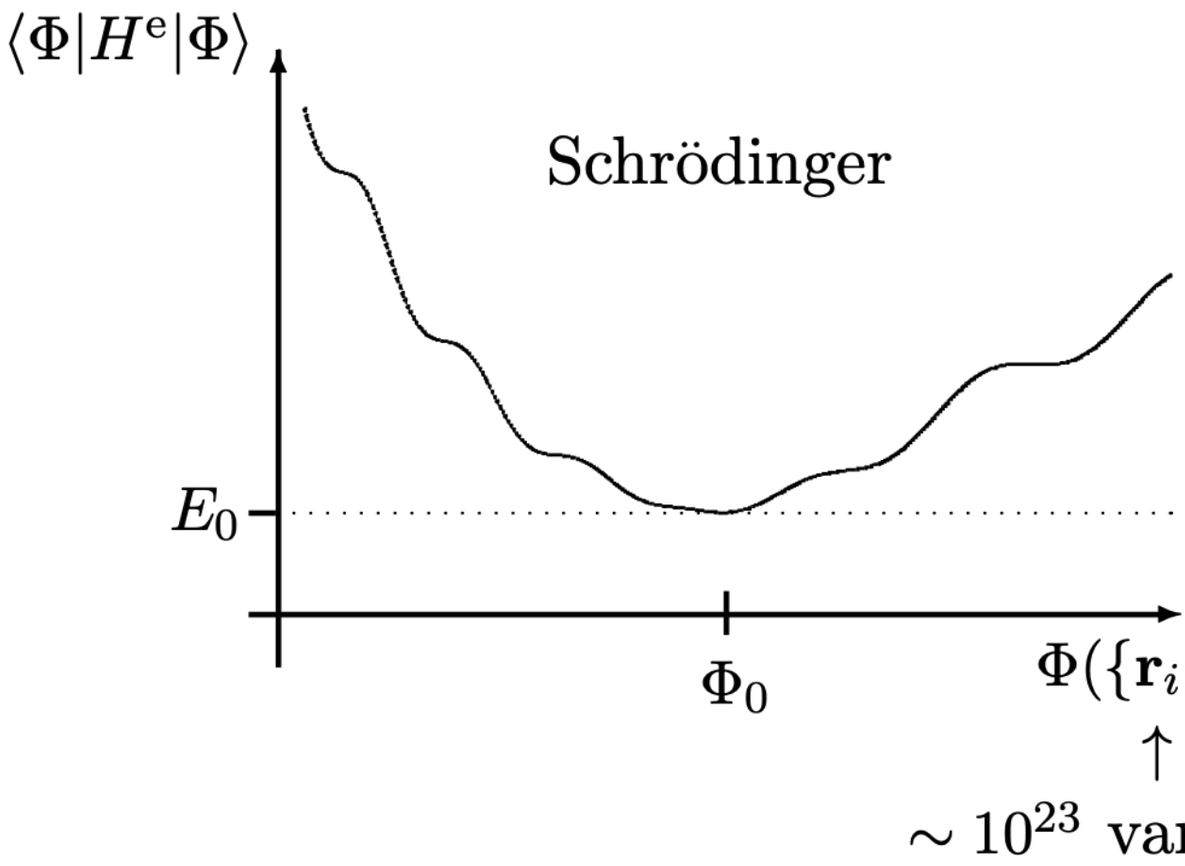
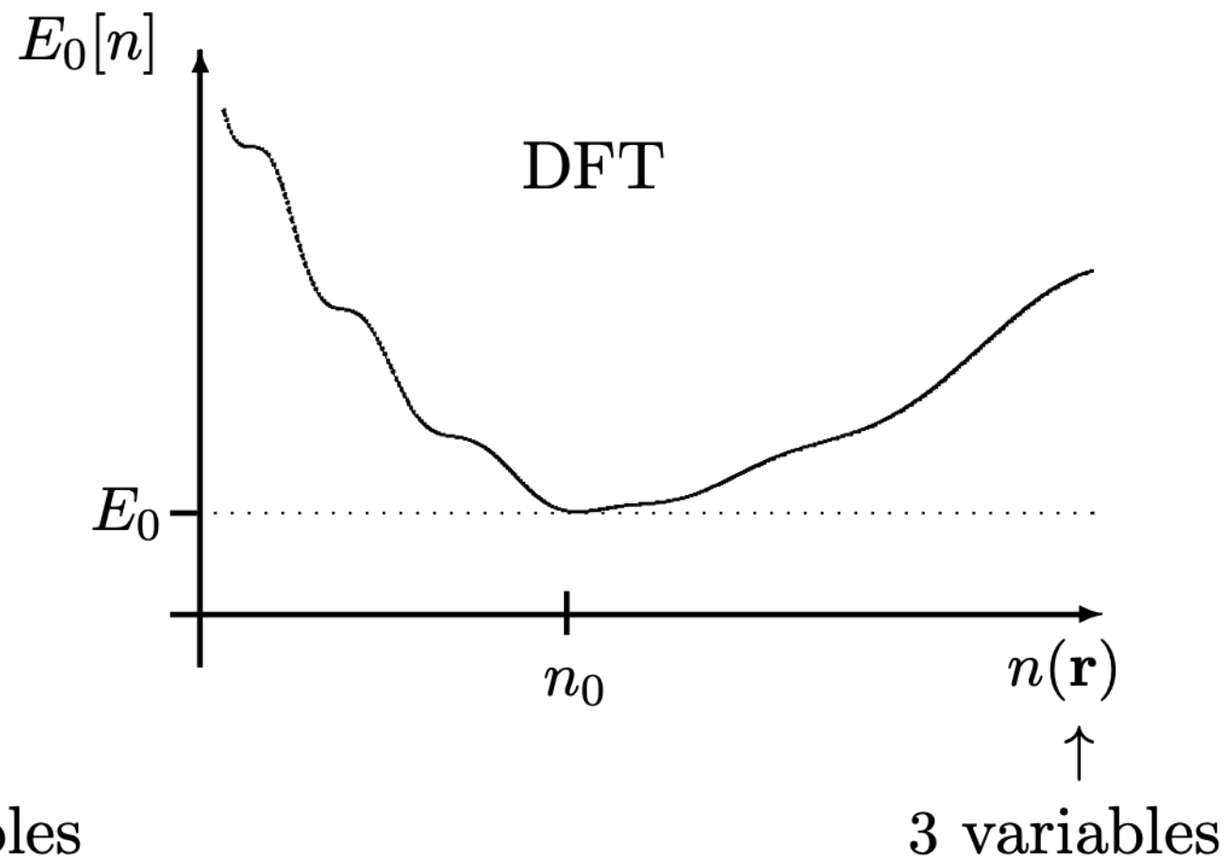
DFT - Variational principle





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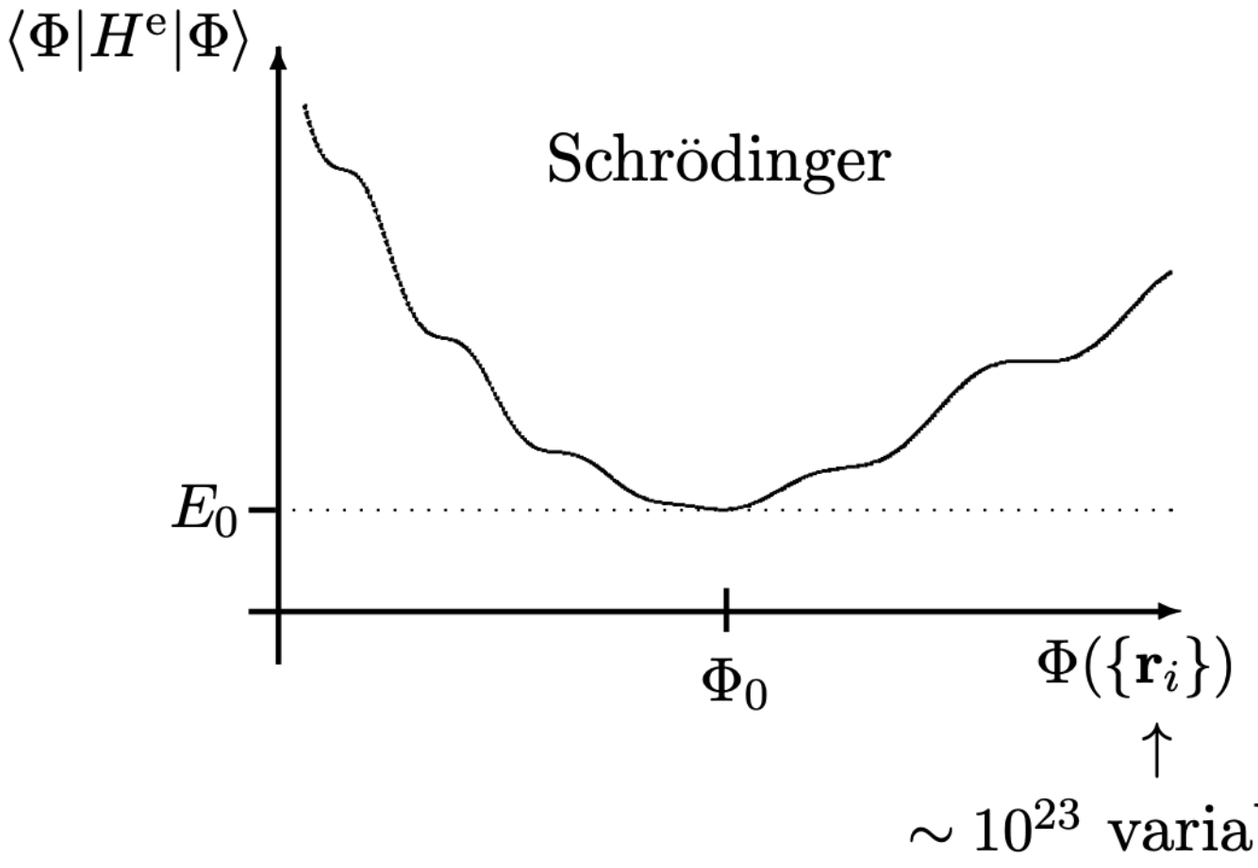

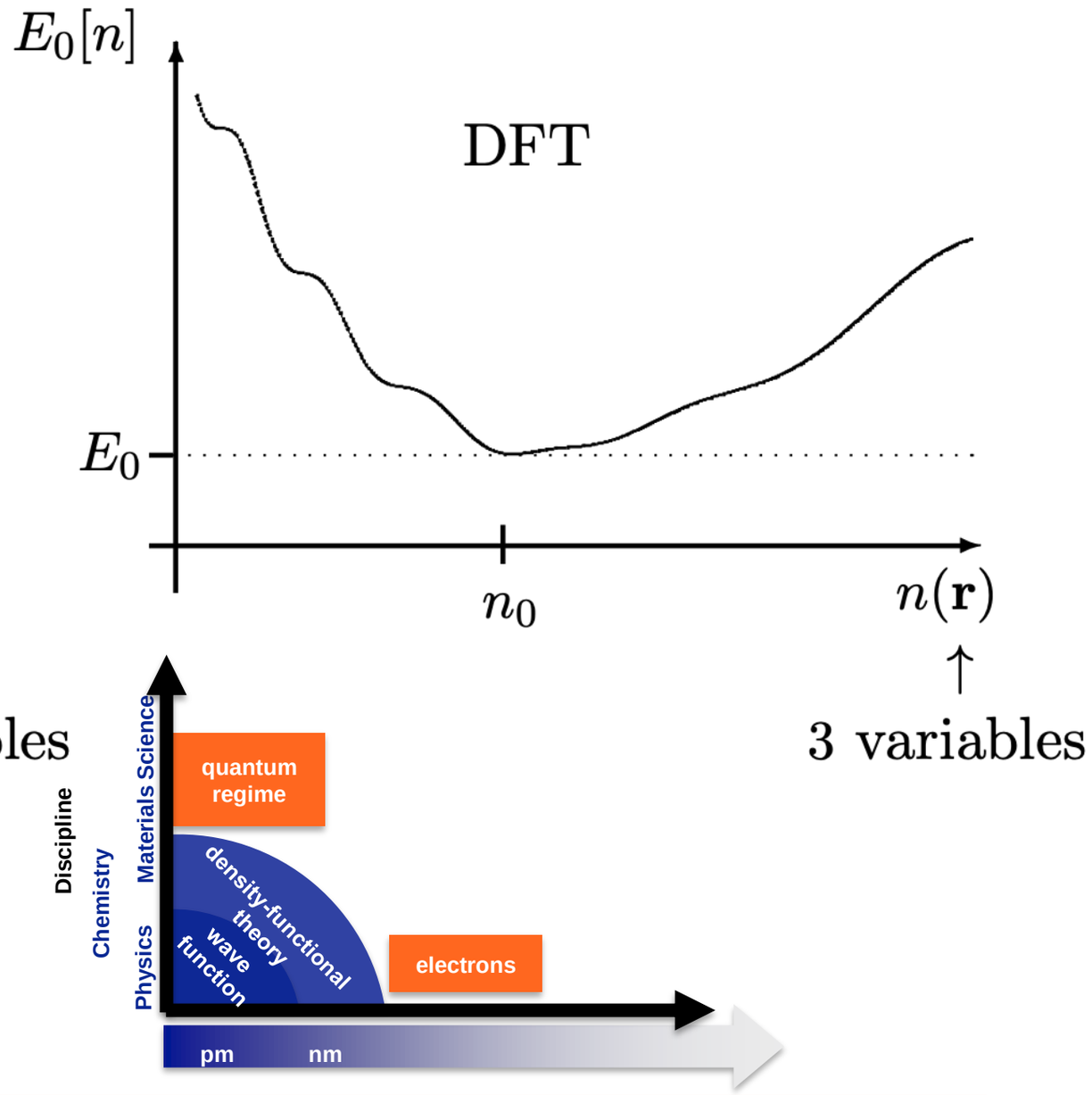

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The three *principles* of DFT

1: DFT is in principle an exact ground state theory.

2: The energy is a functional of the density.
The ground state energy is attained at the ground state density.

We work with this concept in this course.

3: The energy functional needs to be approximated in practice.

The approximations will be subject of the next course in fall 2023.

Questions, comments, ideas?

- Problem with study rights?

- Interesting materials modellings:
  - Quantum chem. in pharmacy: https://youtu.be/9DESulCWbRQ
  - DFT in industry for Quantum Computing: https://quantum.hrl.com/
  - Biology ADP-to-ATP: https://youtu.be/kXpzp4RDGJI
  - FEM microcracs in metals: https://youtu.be/zhIKWleOjBY