capire la natura
e progettare nuovi materiali
usando algoritmi intelligenti e potenti supercomputer

Stefano Baroni

Scuola Internazionale Superiore di Studi Avanzati &
Istituto Officina dei Materiali del CNR, Trieste
QUANTUM ESPRESSO Foundation, Cambridge, UK

lezione presentata al corso *Addressing the Challenges of Digital Innovation: Supercomputing and Business*, Trieste-Bologna, 16-18 marzo 2022

human ages are named after materials:

credit: Nicola Marzari

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- stone

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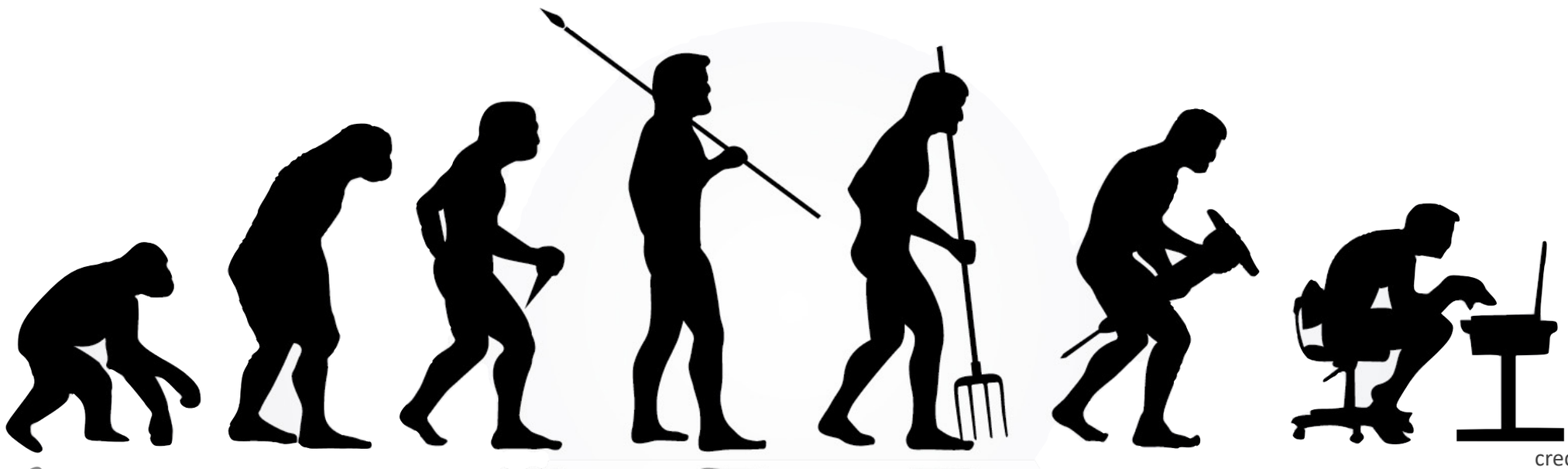
- bronze and iron



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human ages are named after materials:

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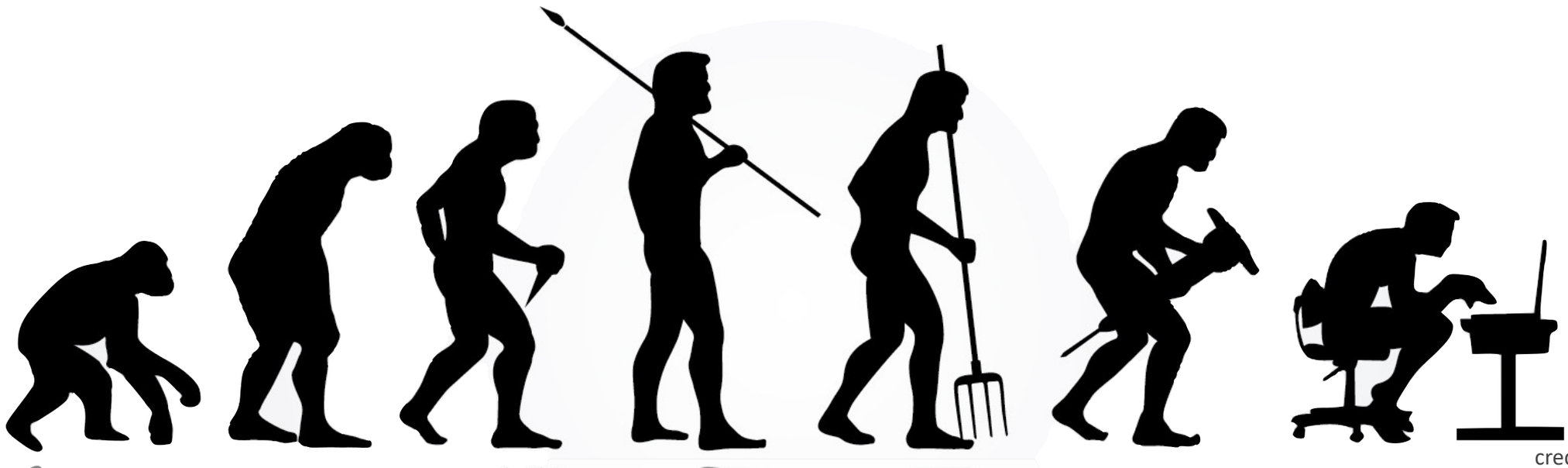

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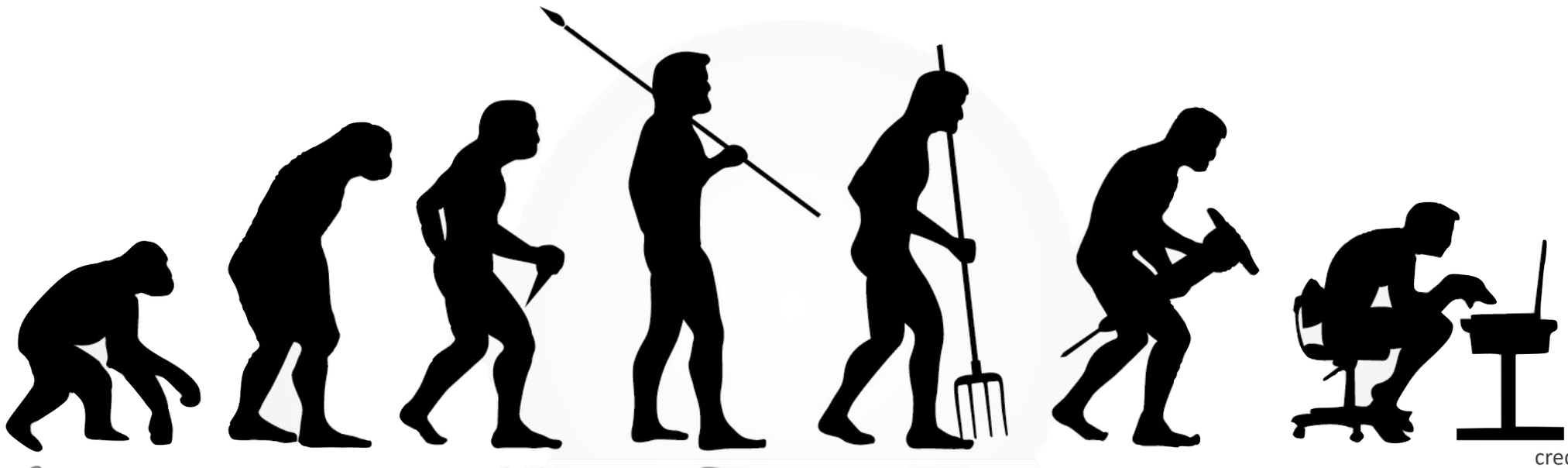

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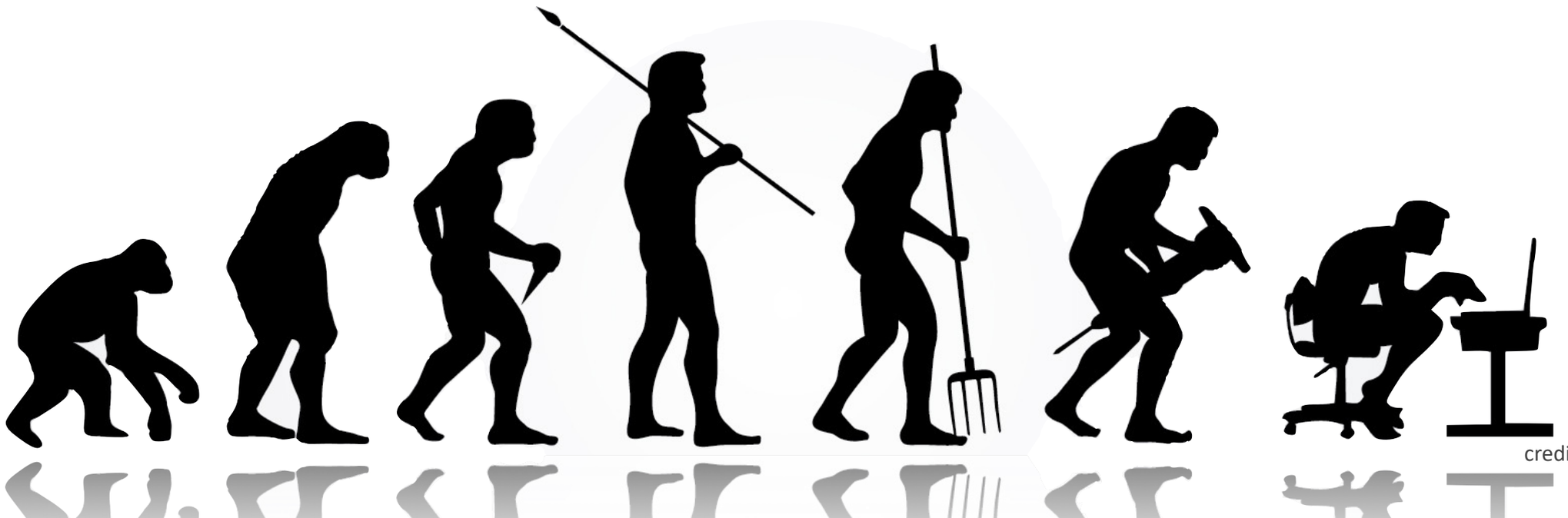

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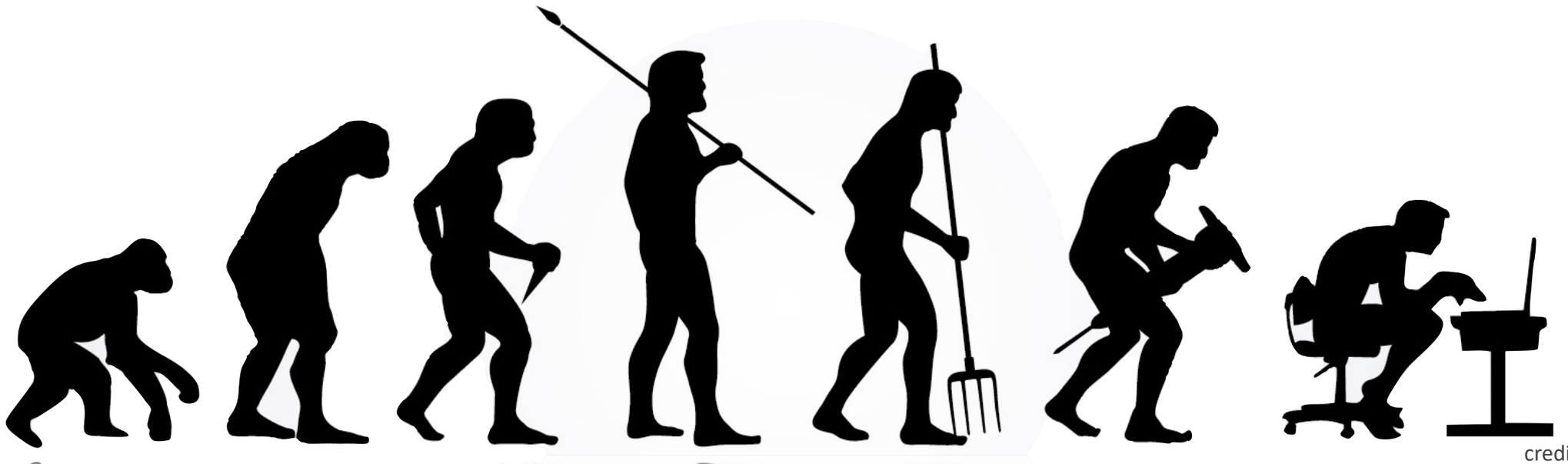
- … what next?



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… societal well being

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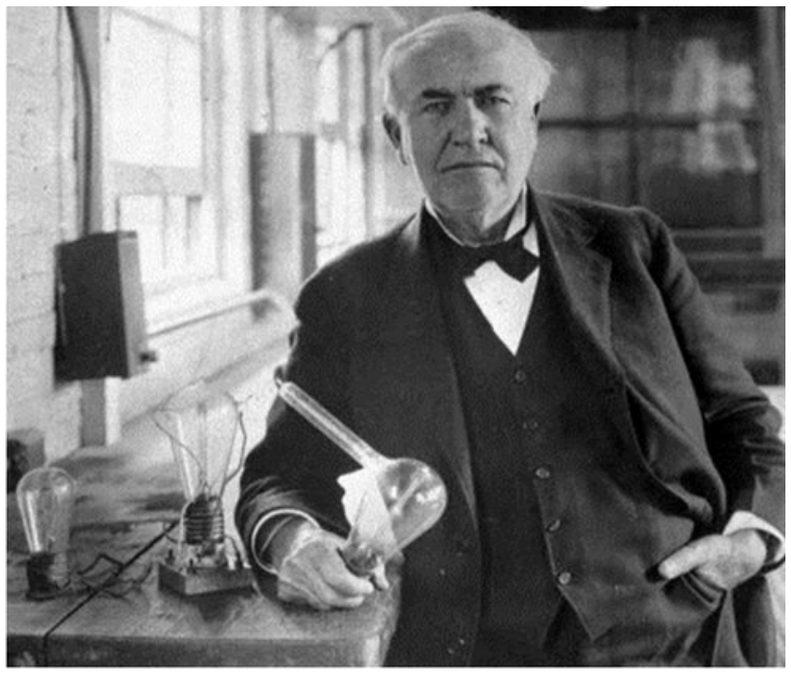

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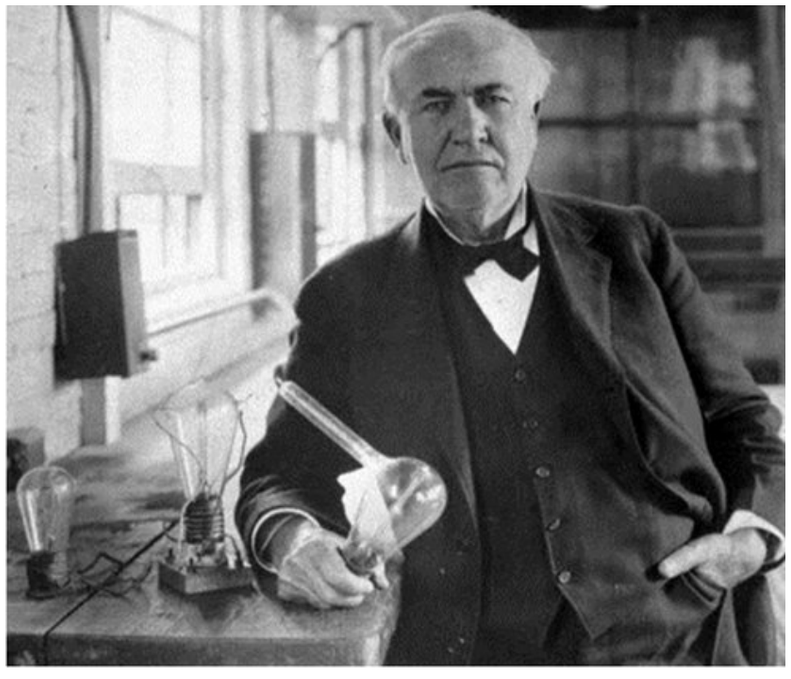
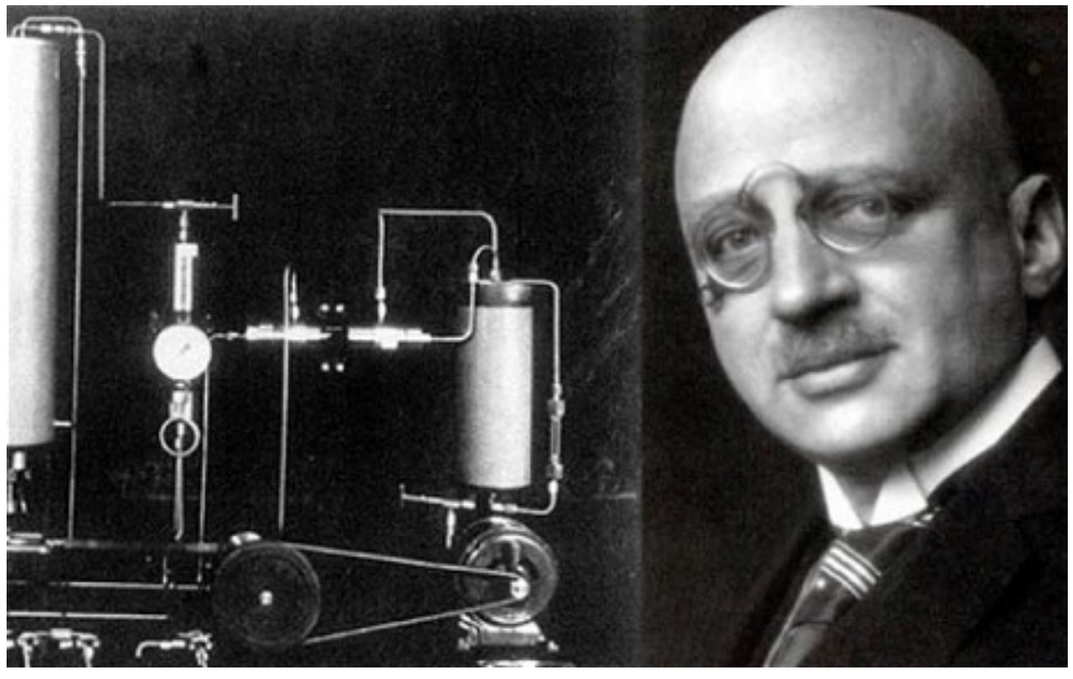
- Haber–Bosch ammonia synthesis used osmium as catalyst. Mittasch (BASF) tested more than 22,000 materials to identify the iron-based catalyst which is still used today.





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quantum mechanics and supercomputers can do more and faster …

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- Using state-of-the-art quantum-mechanical numerical modelling, Norskov showed in 2009 that CoMo is a more efficient and inexpensive catalyst

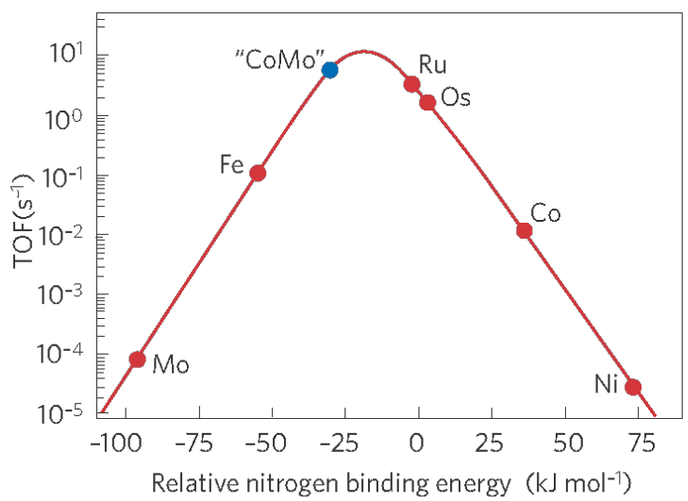
nature chemistry

REVIEW ARTICLE

PUBLISHED ONLINE: 19 MARCH 2009 | DOI: 10.1038/NCHEM.121

Towards the computational design of solid catalysts

J. K. Nørskov[1]*, T. Bligaard[1], J. Rossmeisl[1] and C. H. Christensen[2]



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la teoria quantistica dei materiali

Proc. Roy. Soc. London. Ser A, Vol. 123 (1929)

Quantum Mechanics of Many-Electron Systems.

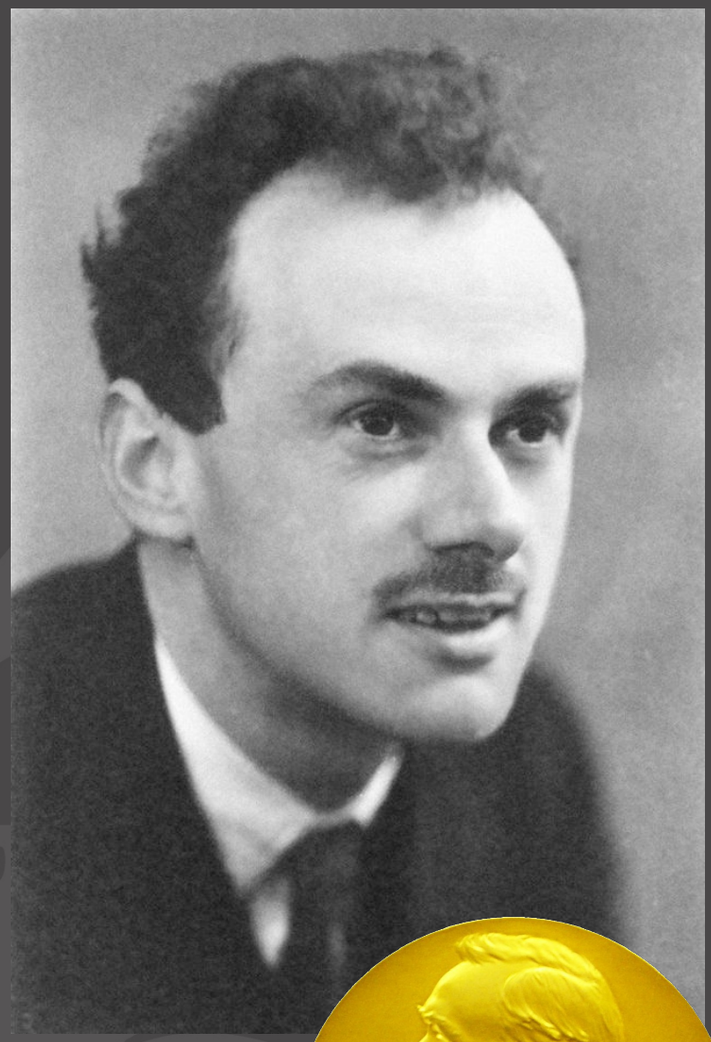
By P. A. M. Dirac, St. John's College, Cambridge.

(Communicated by R. H. Fowler, F.R.S.—Received March 12, 1929.)

§ 1. *Introduction.*

The general theory of quantum mechanics is now almost complete, the imperfections that still remain being in connection with the exact fitting in of the theory with relativity ideas. These give rise to difficulties only when high-speed particles are involved, and are therefore of no importance in the consideration of atomic and molecular structure and ordinary chemical reactions, in which it is, indeed, usually sufficiently accurate if one neglects relativity variation of mass with velocity and assumes only Coulomb forces between the various electrons and atomic nuclei. 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. 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.

Already before the arrival of quantum mechanics there existed a theory of atomic structure, based on Bohr's ideas of quantised orbits, which was fairly



premio Nobel
per la fisica
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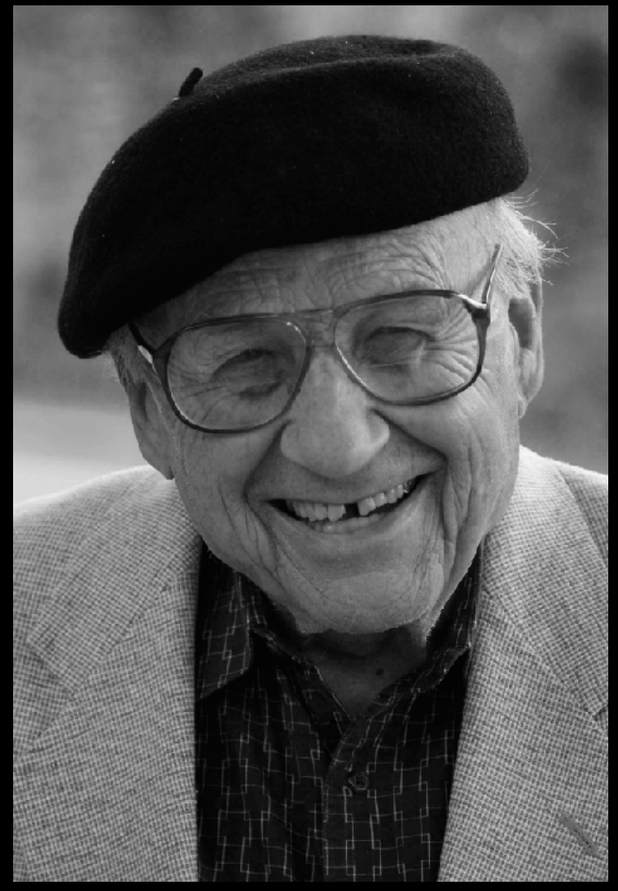

la teoria del funzionale densità

$$\Psi = \Psi(\mathbf{r}_1, \mathbf{r}_2, \cdots \mathbf{r}_N)$$

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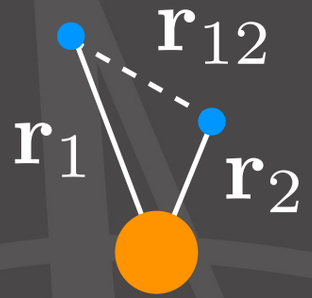

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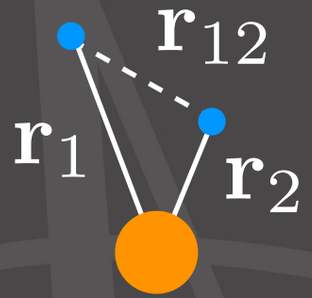

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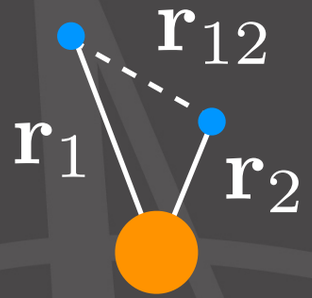

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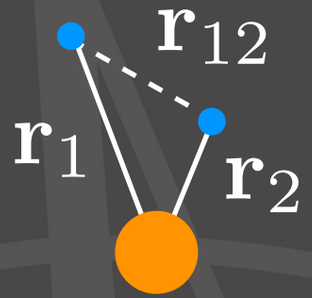

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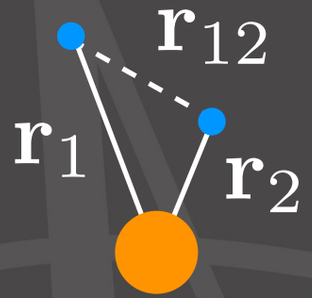

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$$V(\mathbf{r}_1, \mathbf{r}_2) \approx v_n(\mathbf{r}_1) + v_n(\mathbf{r}_2)$$

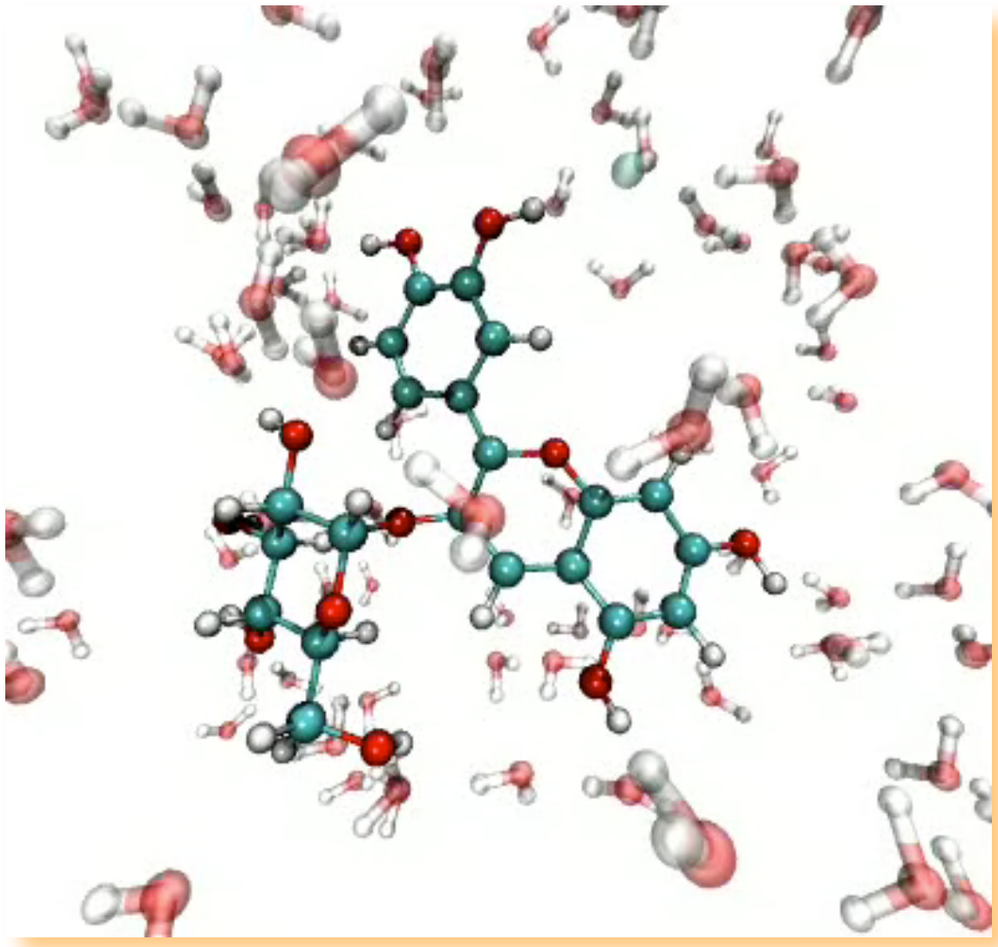
Walter Kohn

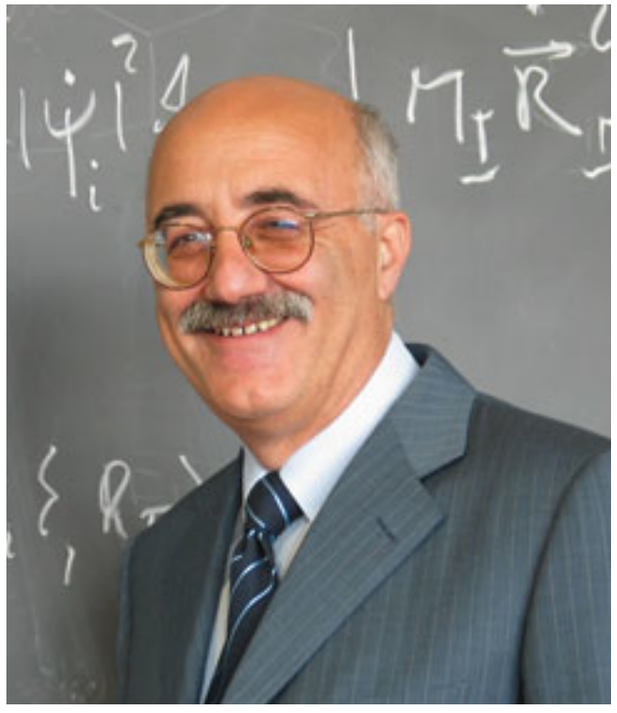
premio Nobel
per la chimica
1999

da Monsieur Daguerre ai fratelli Lumière

la danza infinita degli atomi

Roberto Car e Michele Parrinello
SISSA, 1985





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Dirac medal, 2009
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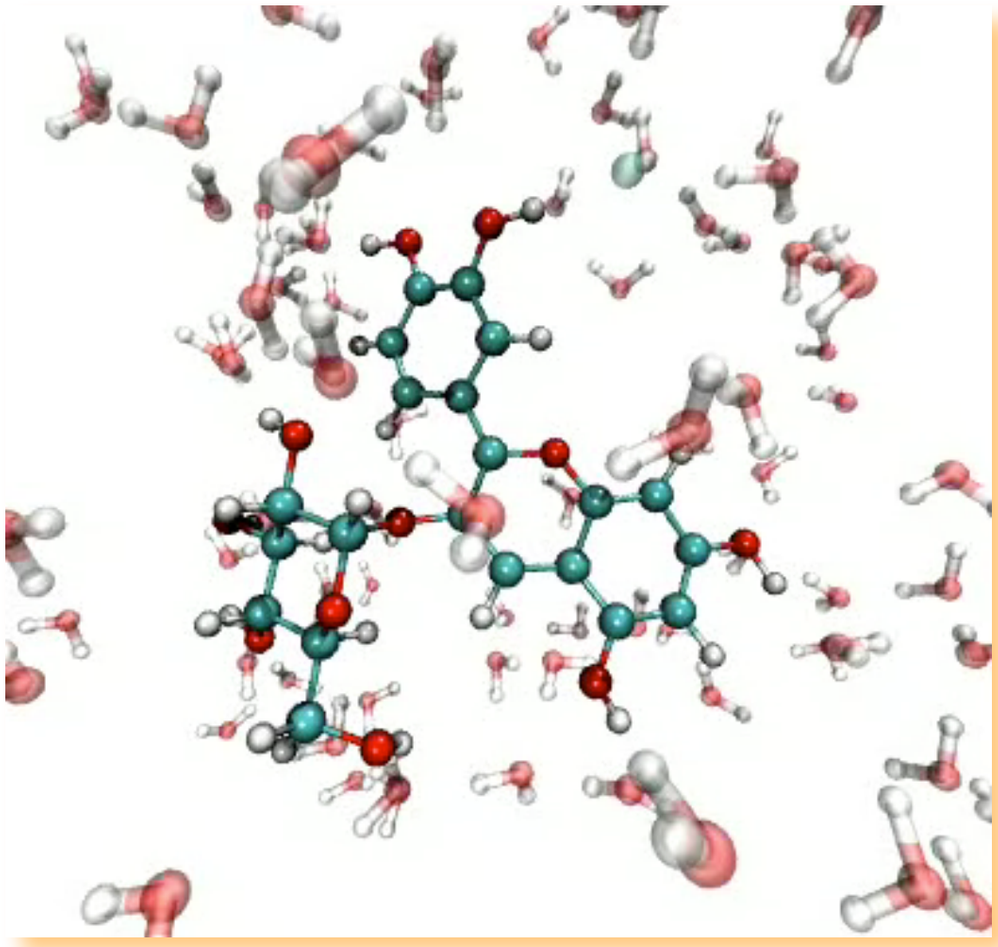

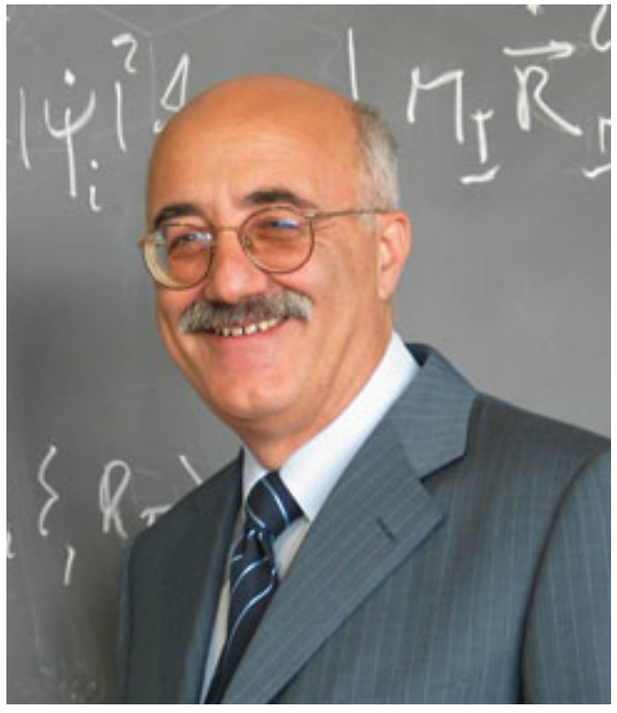

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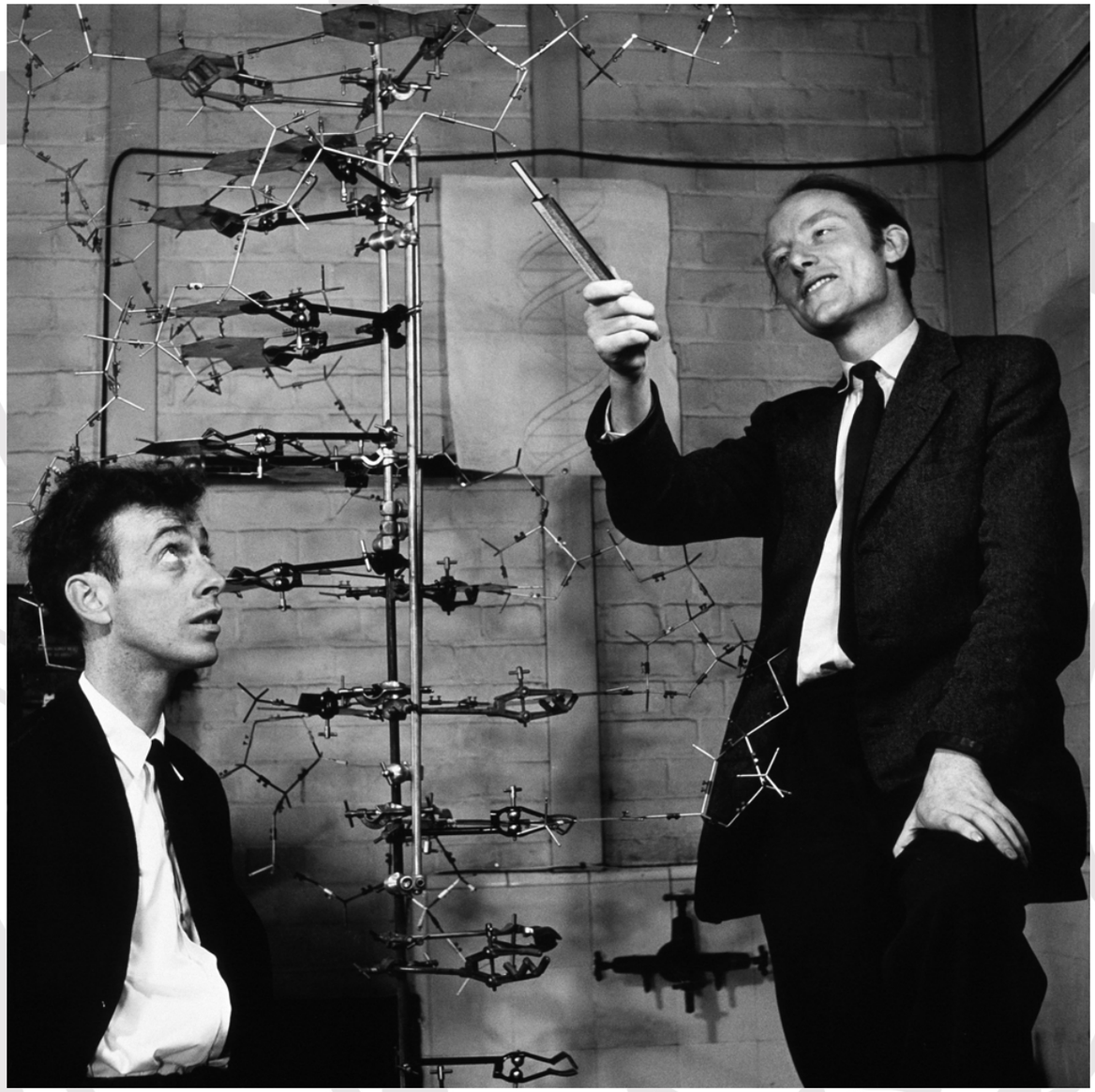

back in the fifties

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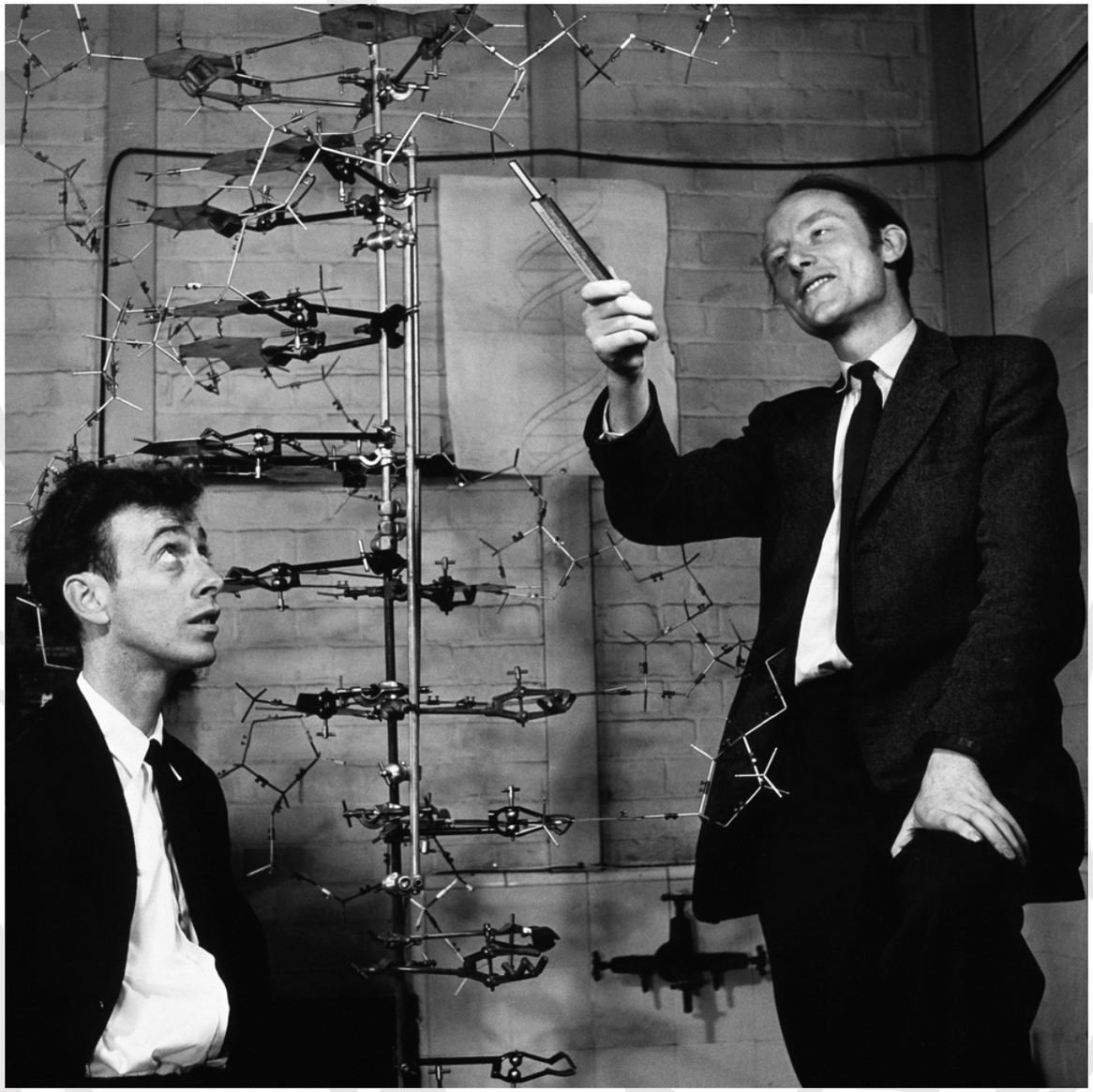

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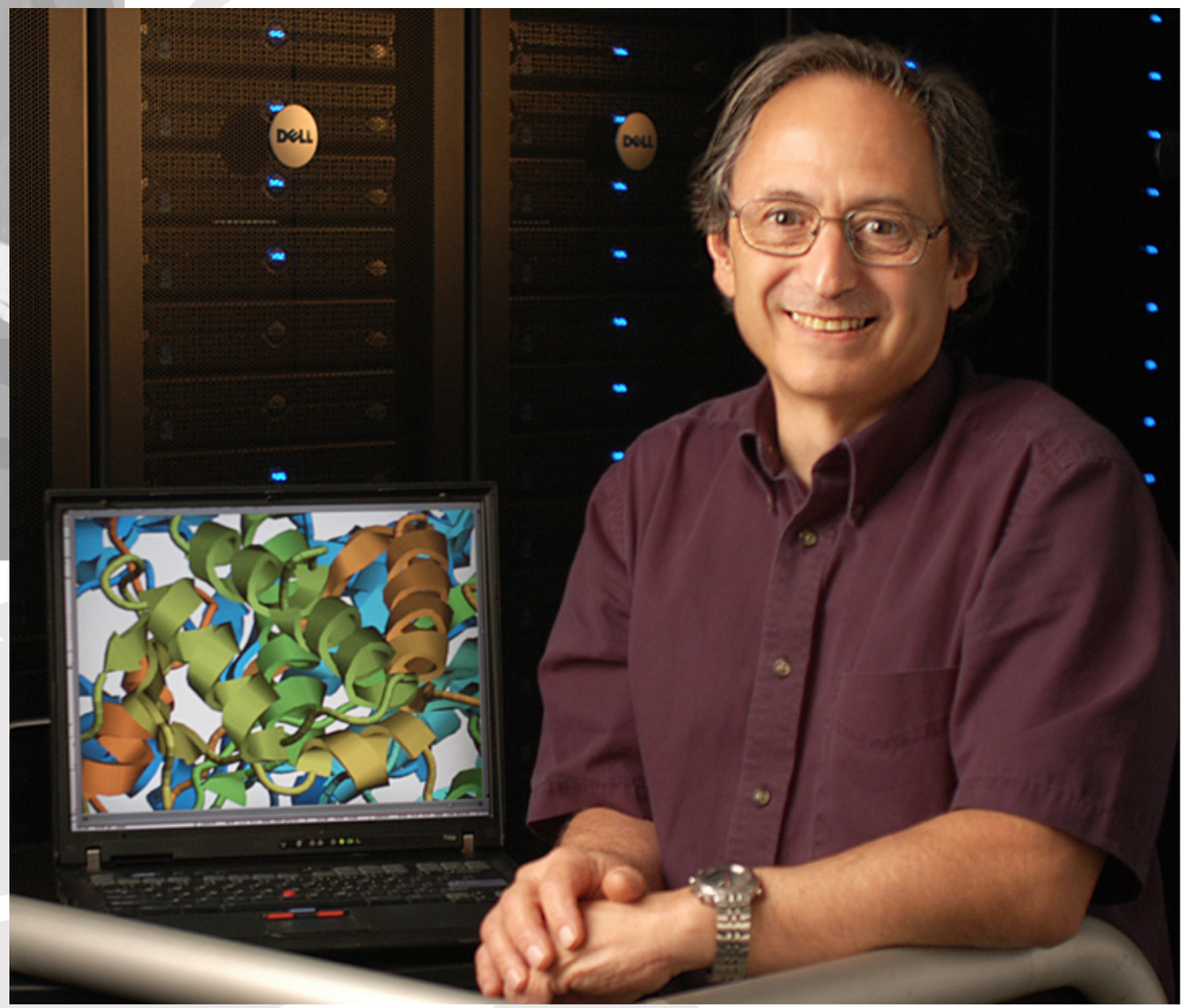
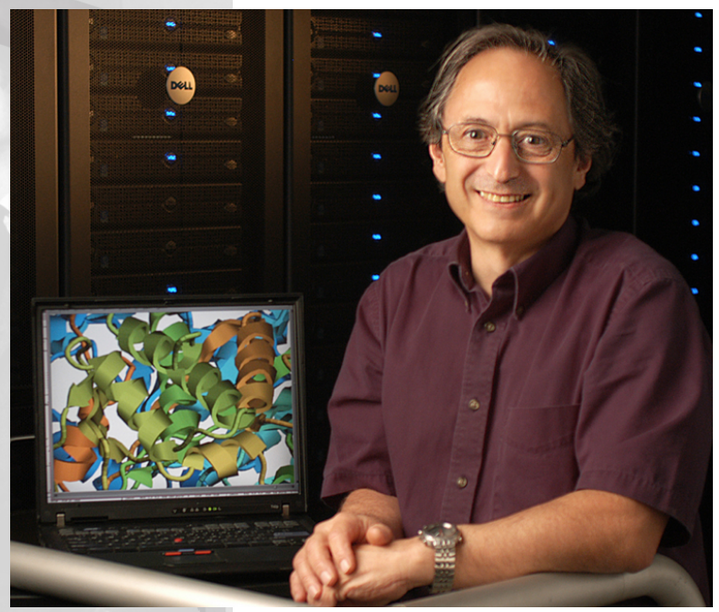


molecular modeling

third millennium

Michael Levitt



2013

"for the development of multiscale [computational] models for complex chemical systems"

back in the fifties

1962

Arieh Warshel

Martin Karplus

QUANTUMESPRESSO

what is QUANTUM ESPRESSO?

QUANTUM ESPRESSO is an integrated suite of computer codes for atomistic simulations based on DFT, pseudo-potentials, and plane waves

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what is QUANTUM ESPRESSO?

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QUANTUM ESPRESSO is an initiative coordinated by the QUANTUM ESPRESSO Foundation, with the participation of SISSA, CNR, UniUD, CINECA, ICTP, EPFL, the University of Texas at Austin, with many partners in Europe and worldwide

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QUANTUM ESPRESSO is not a single application for quantum simulations; it is rather a distribution of packages performing different tasks and designed to be interoperable

QUANTUM ESPRESSO is *free* software that can be *freely* downloaded. Everybody is *free* to use it and welcome to contribute to its development

QUANTUM ESPRESSO in numbers

- ≈ 300,000+ lines of FORTRAN/C code
- ≈ 60 developers registered oh GitLab/Hub
- 3000+ registered users
- 4000+ downloads for each new release
- 2000+ scientific papers per year
- 2 web sites (quantum-espresso.org, foundation@quantum-espresso.org)
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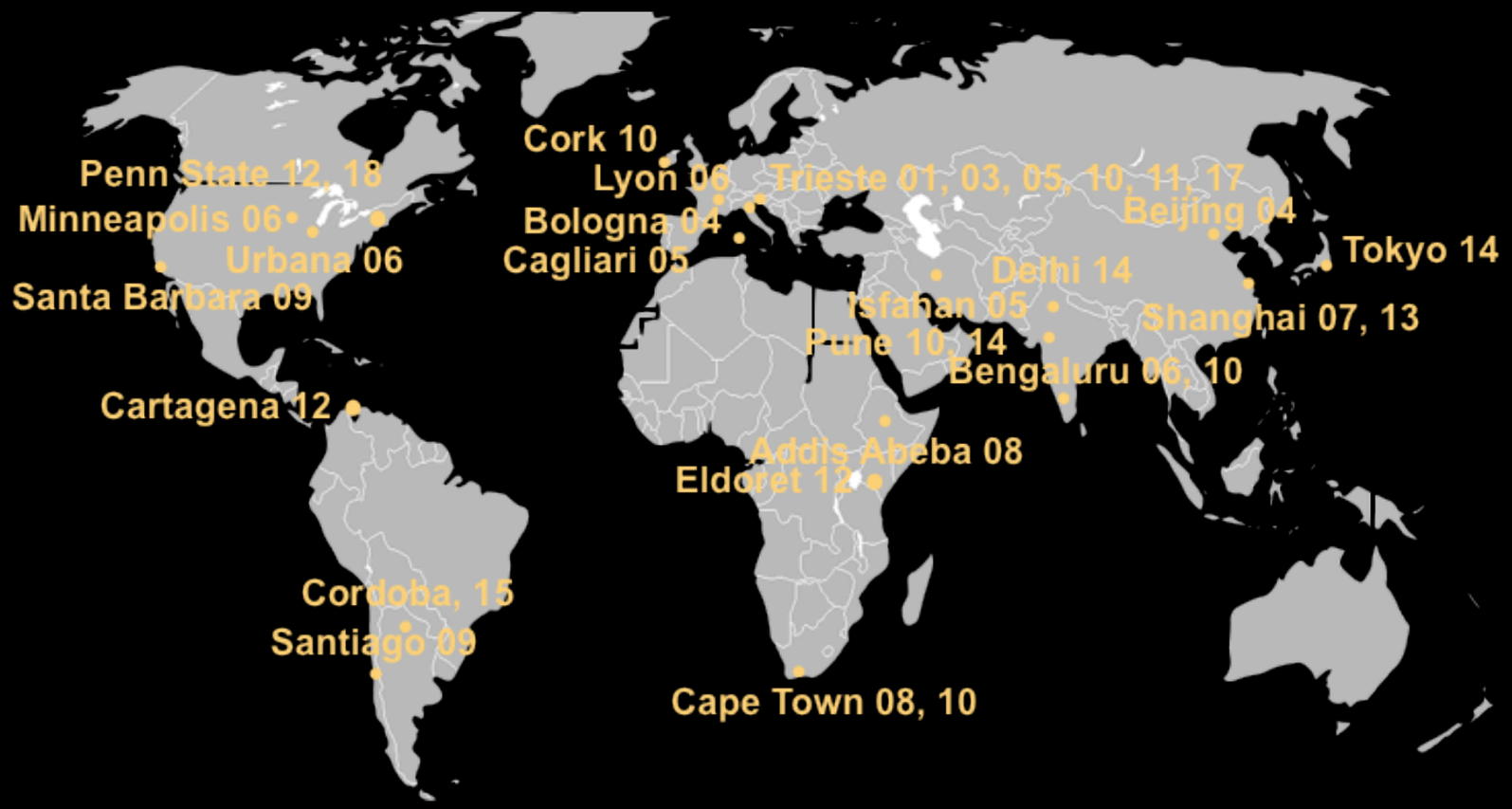
- 1 popular international web discussion forum
- ≈ 40 international schools and training courses since 2001 (2000+ participants worldwide)



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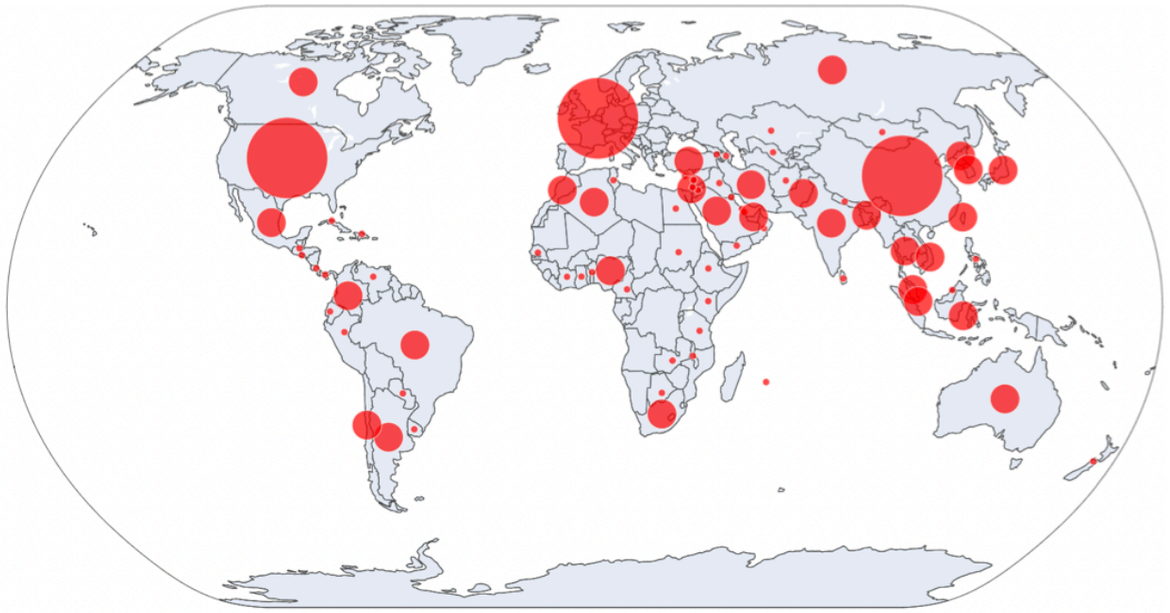
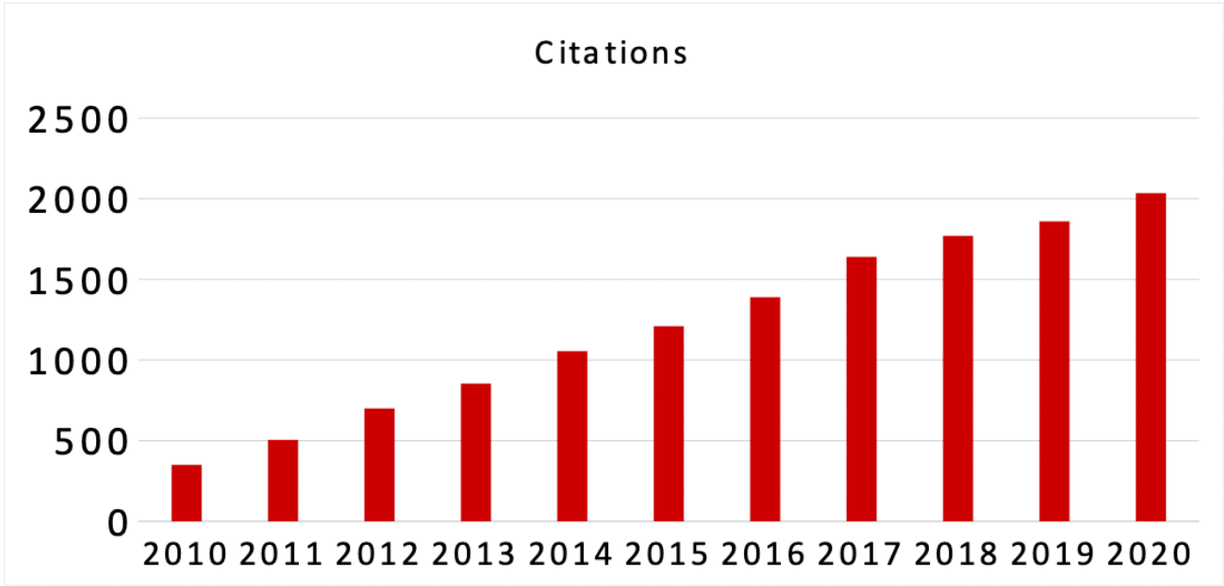
chi usa QUANTUM ESPRESSO?

Worldwide as of 2021 ~25k researchers



Europe 35% USA 22% China 14%

Numbers of successful researches



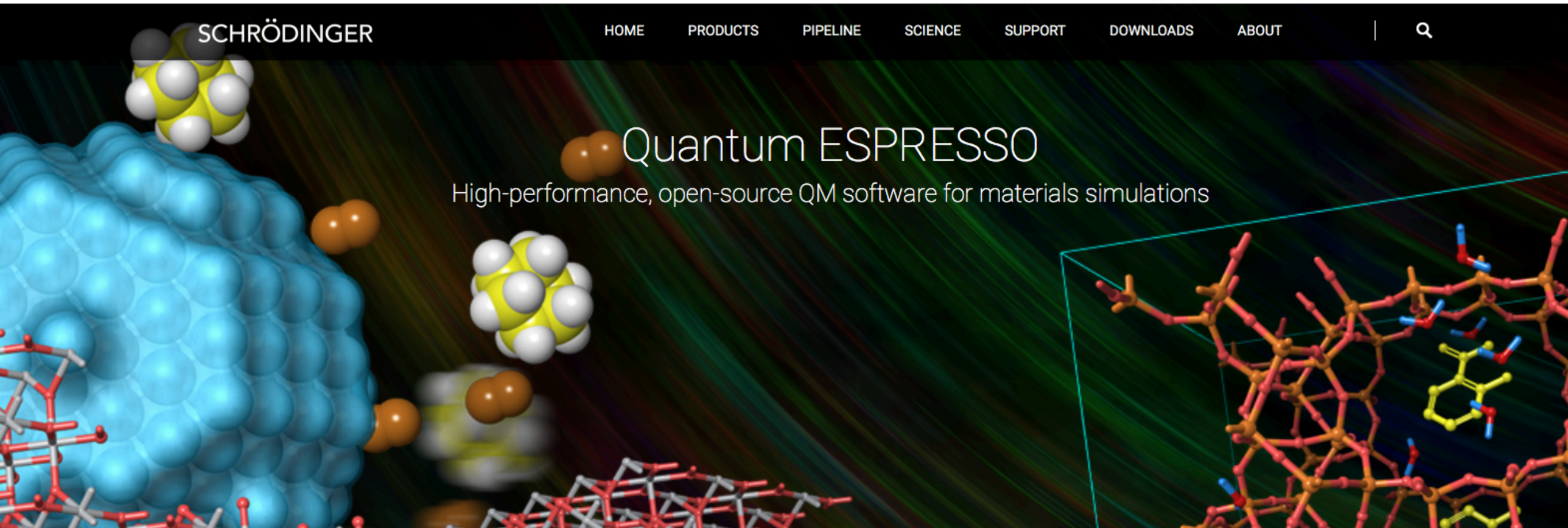
~ 15k publications

QUANTUM ESPRESSO goes to the market

Schrödinger Inc. and the **Quantum ESPRESSO Foundation** announce an on-going development collaboration to integrate the QUANTUM ESPRESSO materials simulation program into the Schrödinger modelling suite

SCHRÖDINGER

QUANTUM ESPRESSO FOUNDATION



$$-\frac{\hbar^2}{2m}\Delta\Psi_n(x)+V(x)\Psi_n(x)=E_n\Psi_n(x)$$

quantum mechanics on a supermarket shelf

how digital computers helped apply theoretical physics to chocolate candies

the food industry is subject to an increasing global pressure from customers and legislators who demand a shift towards ingredients and additives that are perceived as *more natural* and, “therefore”, *healthier*

the Southampton six

In 2007 Research funded by the UK FSA was published, suggesting that consumption of mixes of certain artificial food colours and the preservative sodium benzoate could be linked to attention deficit and increased hyperactivity in some children.

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Box A: <u>The Seven Southampton Additives</u>

Colours:

Tartrazine (E102)

Quinoline yellow (E104)

Sunset yellow (E110)

Carmoisine (E122)

Ponceau 4R (E124)

Allura red (E129)

Preservative:

Sodium benzoate (E211)

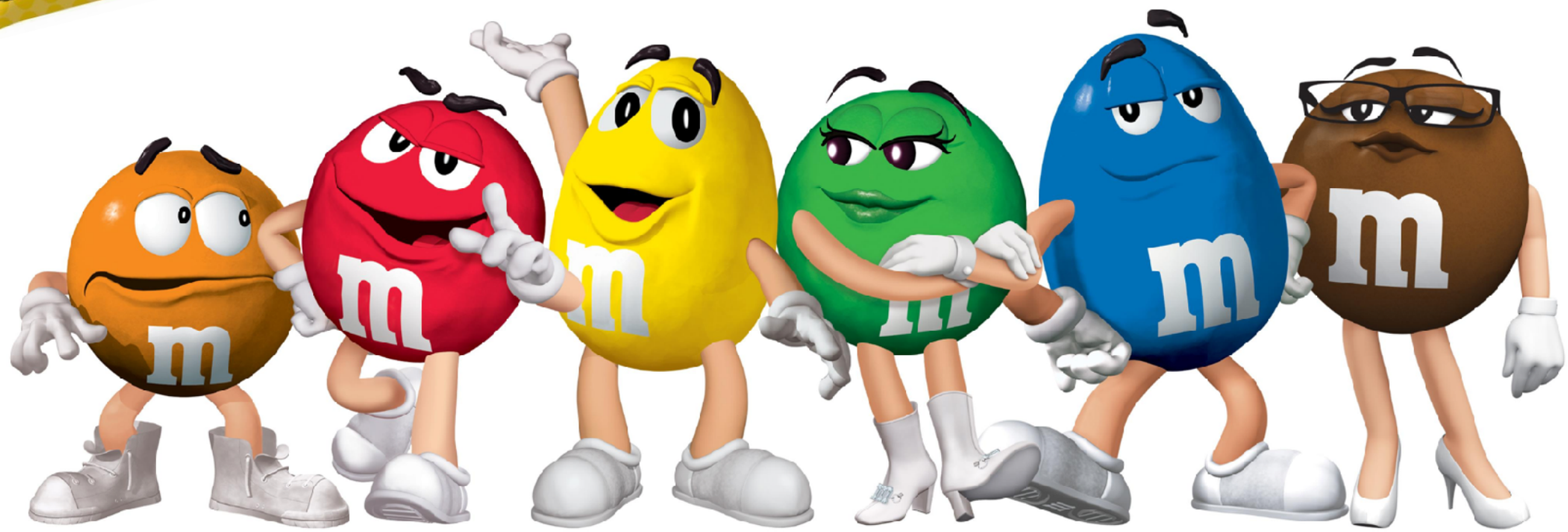
Since 2010 an EU-wide compulsory warning must be put on any food and drink product that contains any of these six colours:

"May have an adverse effect on activity and attention in children"

MARS

chocolate

north america



MARS

chocolate

north america

natural dyes: the requirements

natural dyes: the requirements

- tunable

natural dyes: the requirements

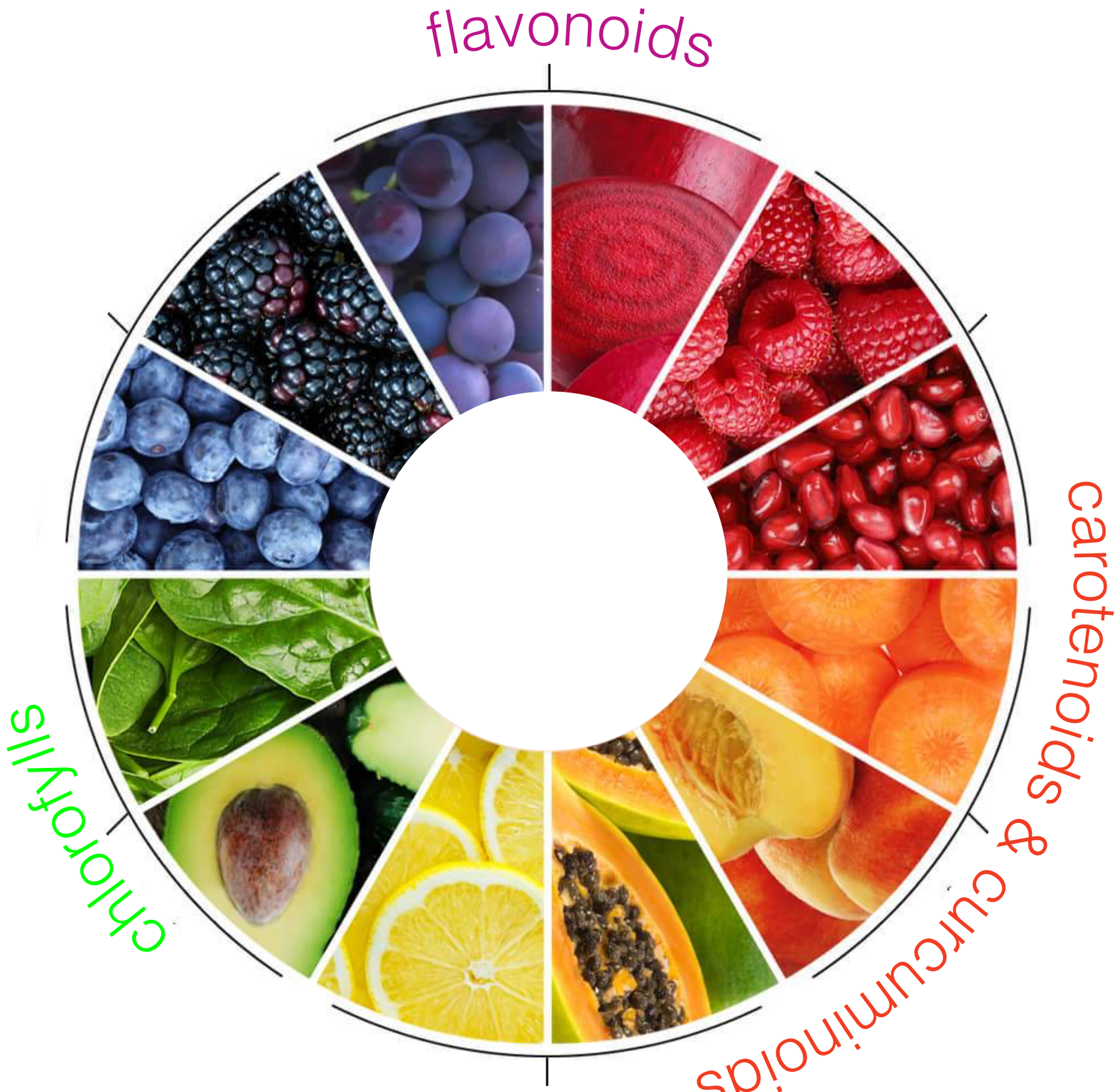
- tunable
- stable

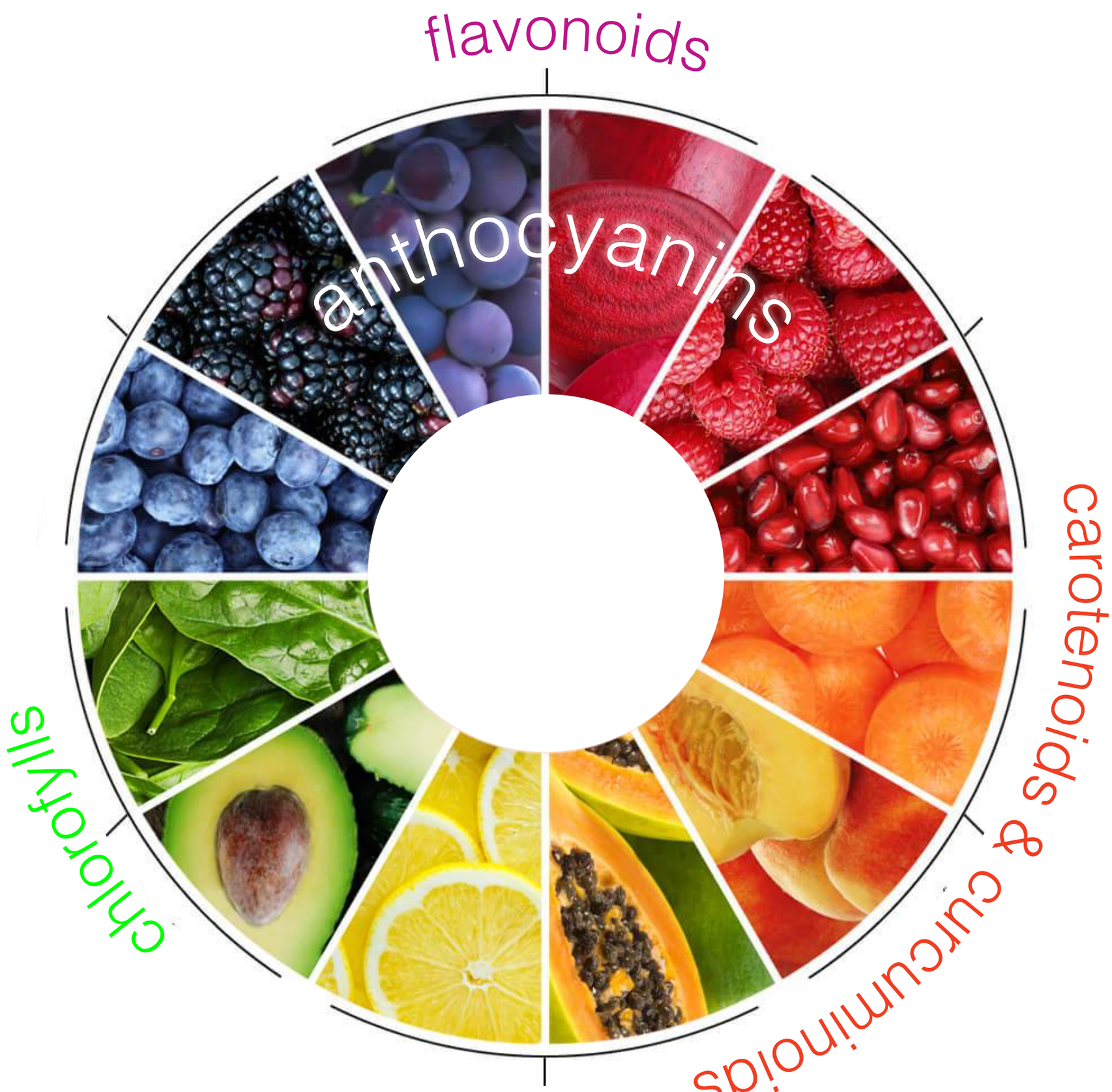
natural dyes: the requirements

- tunable
- stable
- safe

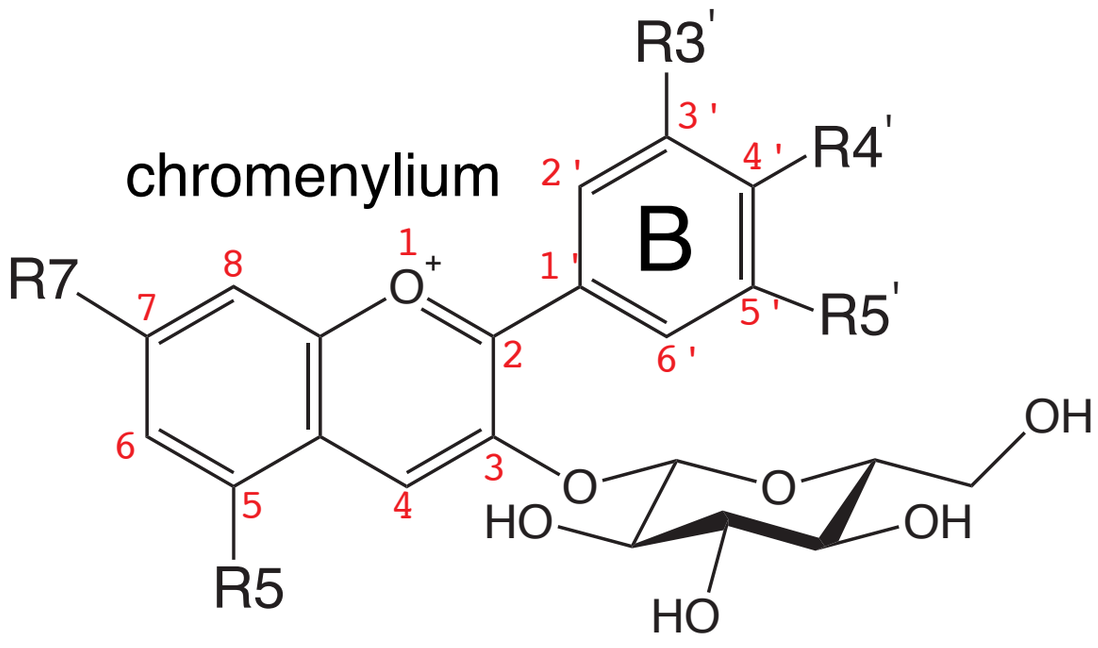
natural dyes: the requirements

- tunable
- stable
- safe
- inexpensive


flavonoids
carotenoids & curcuminoids
chlorophylls

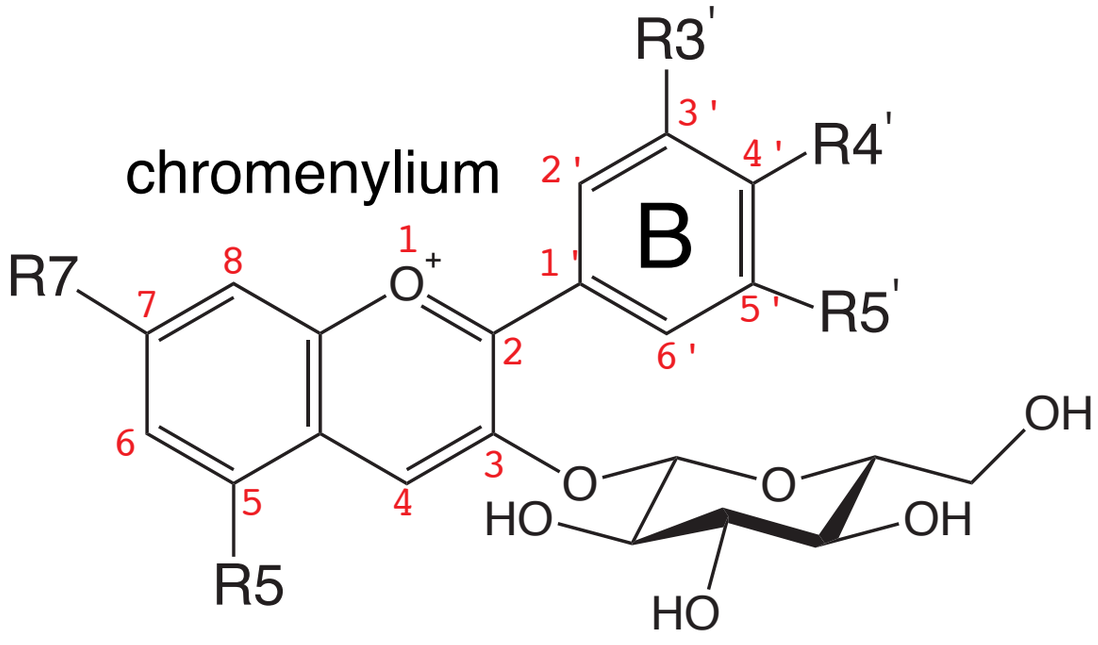

flavonoids
anthocyanins
carotenoids & curcuminoids
chlorophylls

anthocyanins



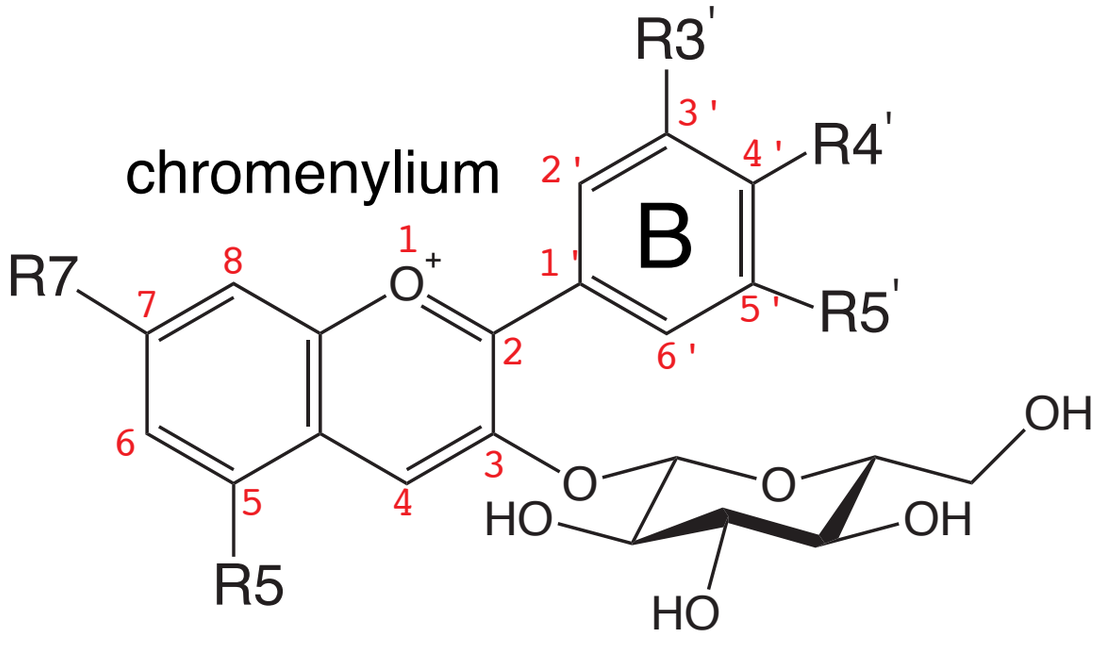
anthocyanin	R3’	R4’	R5’	R7
cyanin	–OH	–OH	–H	–OH

anthocyanins



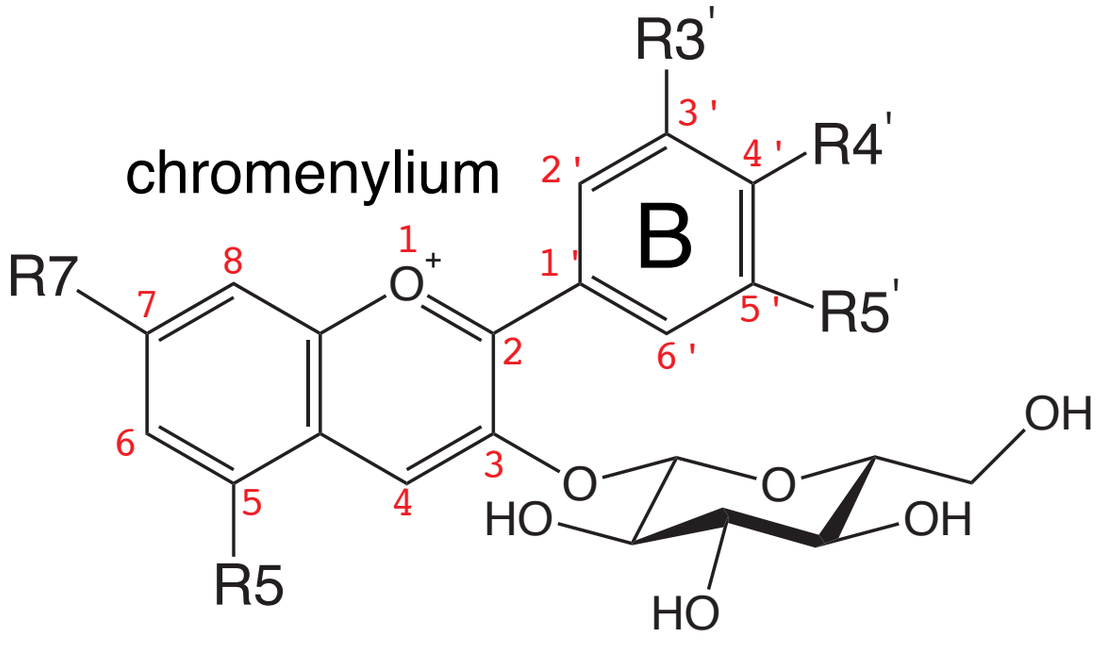
anthocyanin	R3’	R4’	R5’	R7
cyanin	–OH	–OH	–H	–OH
peonin	$–OCH_3$	–OH	–H	–OH

anthocyanins



anthocyanin	R3’	R4’	R5’	R7
cyanin	–OH	–OH	–H	–OH
peonin	$–OCH_3$	–OH	–H	–OH
rosinin	–OH	–OH	–H	$–OCH_3$

anthocyanins



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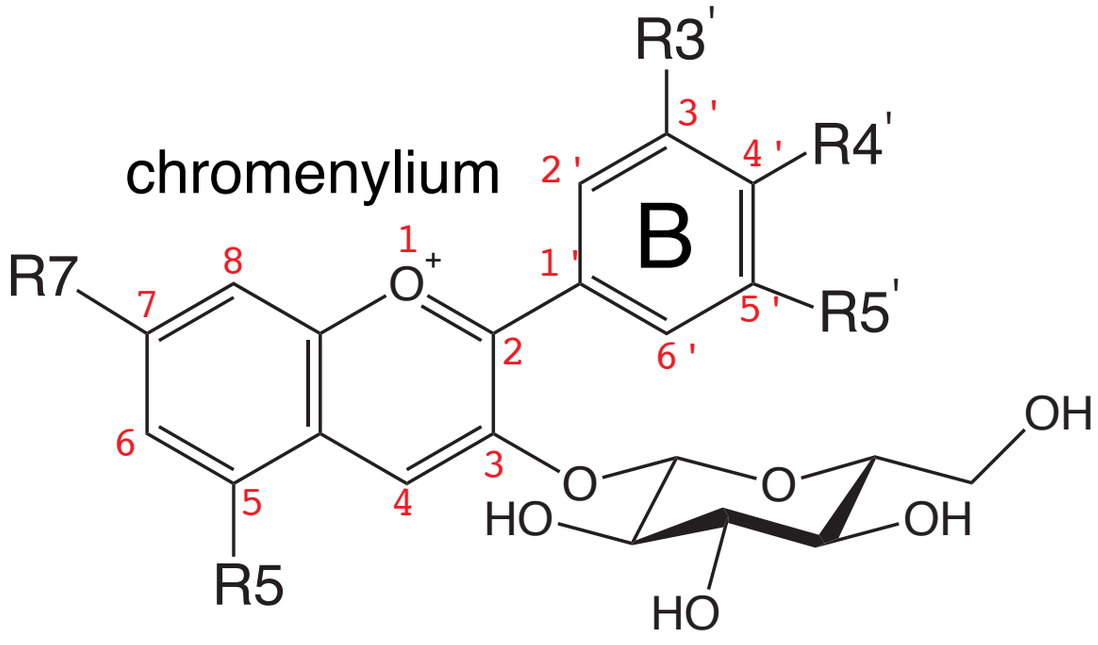
rosinin	–OH	–OH	–H	$–OCH_3$
malvin	$–OCH_3$	–OH	$–OCH_3$	–OH

anthocyanins



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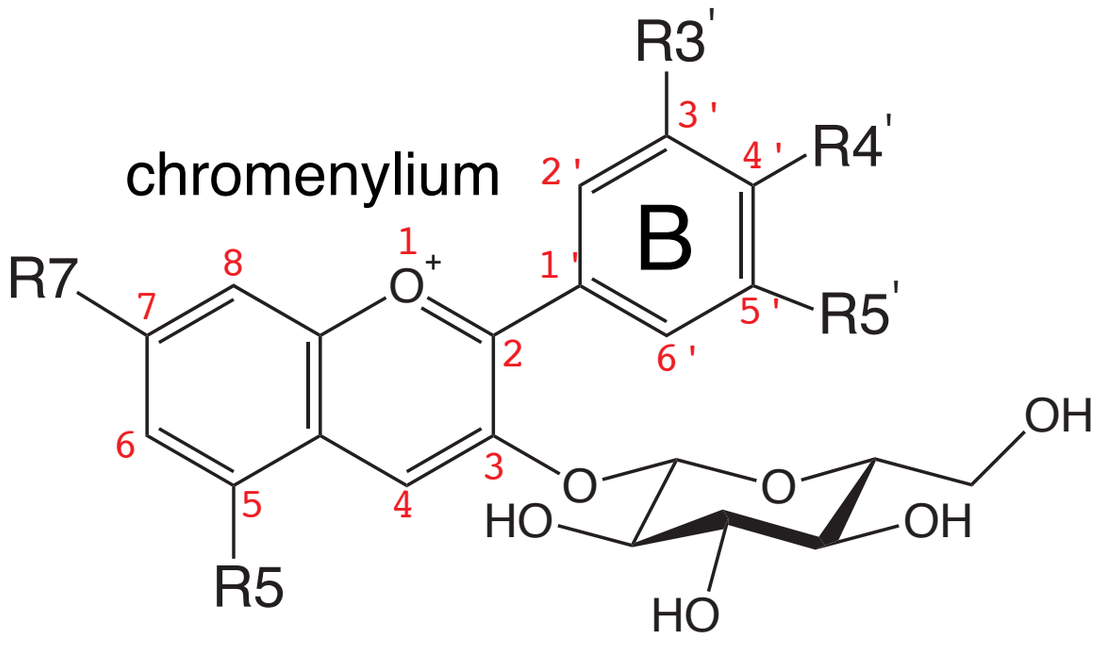
rosinin	–OH	–OH	–H	$–OCH_3$
malvin	$–OCH_3$	–OH	$–OCH_3$	–OH
delphinin	–OH	–OH	$–OCH_3$	–OH

anthocyanins



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peonin	$-OCH_3$	–OH	–H	–OH
rosinin	–OH	–OH	–H	$-OCH_3$
malvin	$-OCH_3$	–OH	$-OCH_3$	–OH
delphinin	–OH	–OH	$-OCH_3$	–OH
pelargonin	–H	–OH	–OH	–OH

anthocyanin: the hurdles towards a rational design

anthocyanin: the hurdles towards a rational design

- the stability and color function of anthocyanins are affected by many and diverse factors:
  - chemical diversity (phenols, sugars, and acylation);
  - acidity of the solution;
  - co-pigmentation;

anthocyanin: the hurdles towards a rational design

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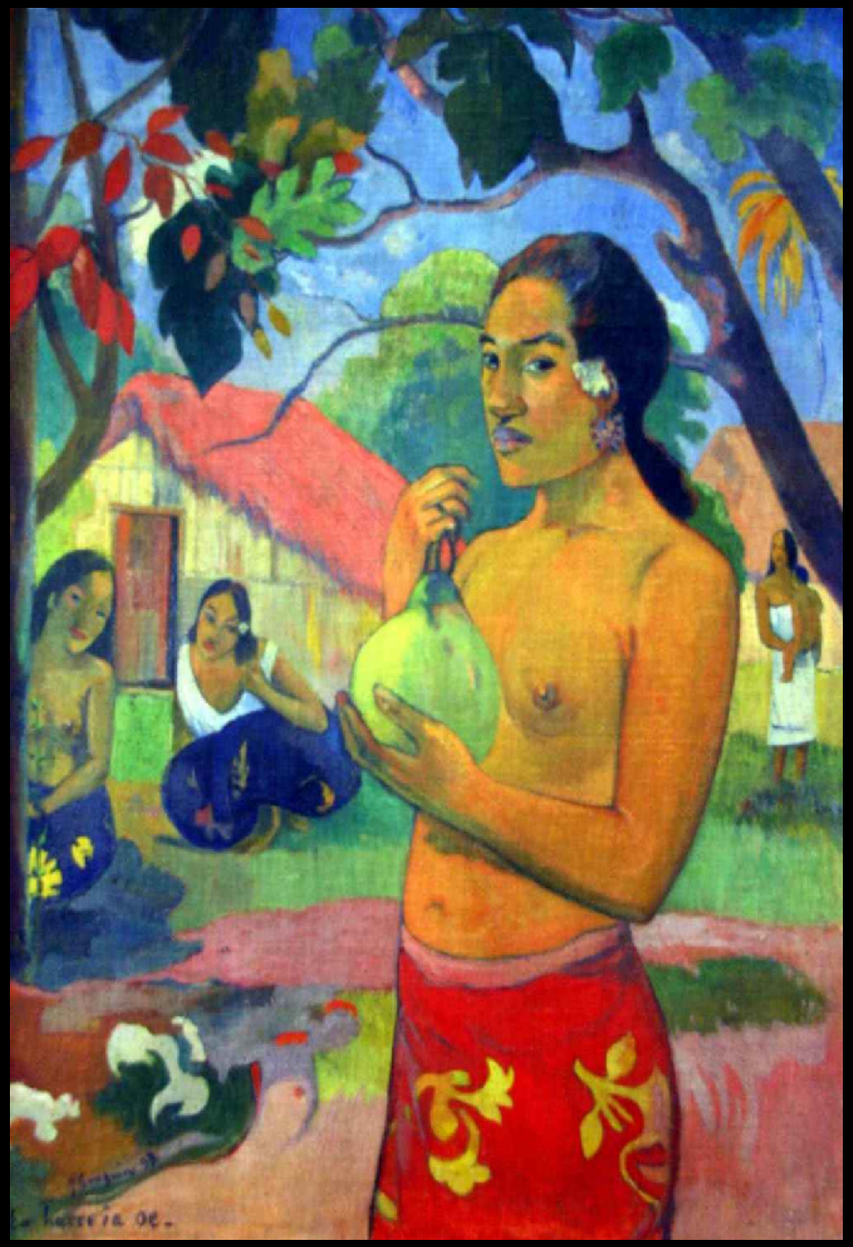
  - very little research is being done in this area;
  - most of it simply aims at isolating from natural sources (highly expensive and difficult);
- very little is known of the microscopic mechanisms that determine the stability and the chromatic properties of anthocyanins and the relation between structure and color.

what color is all about



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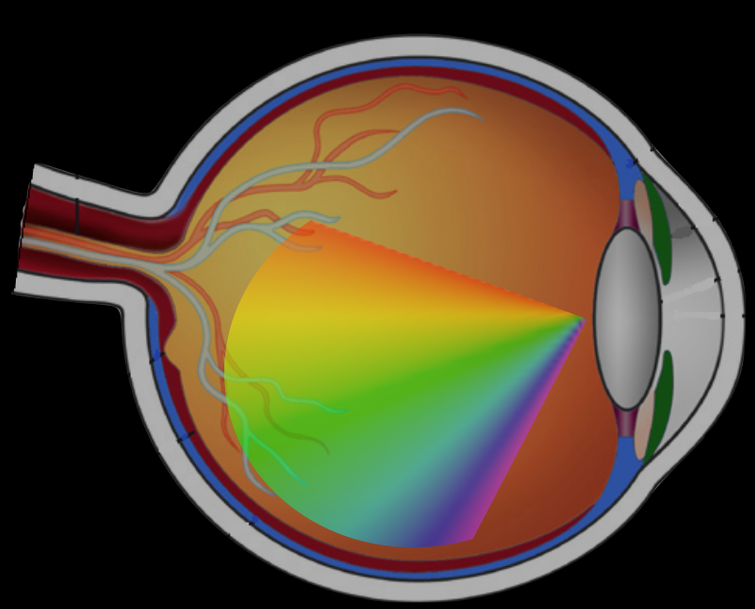
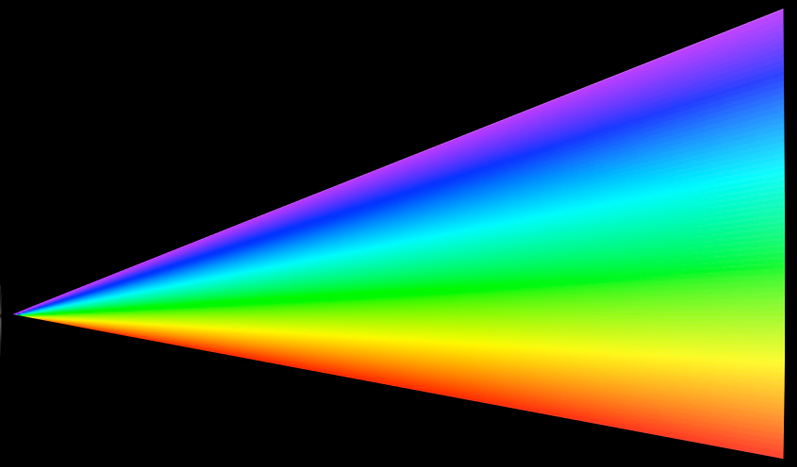
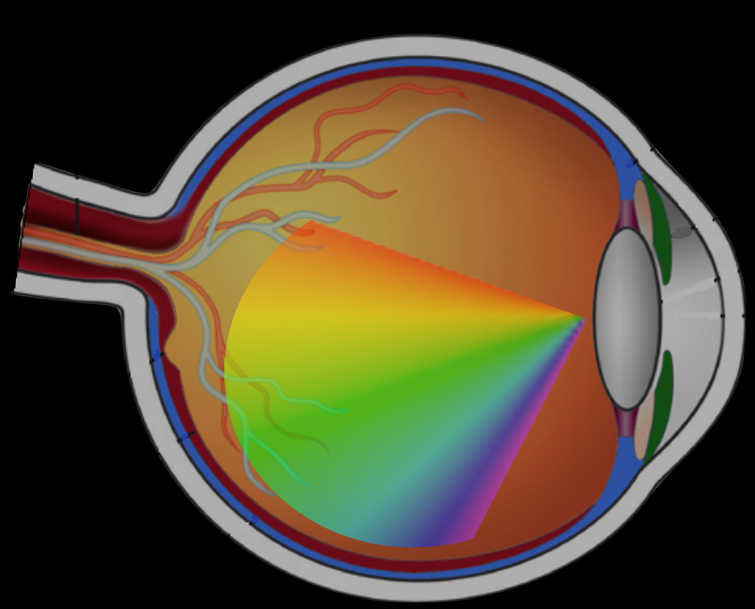
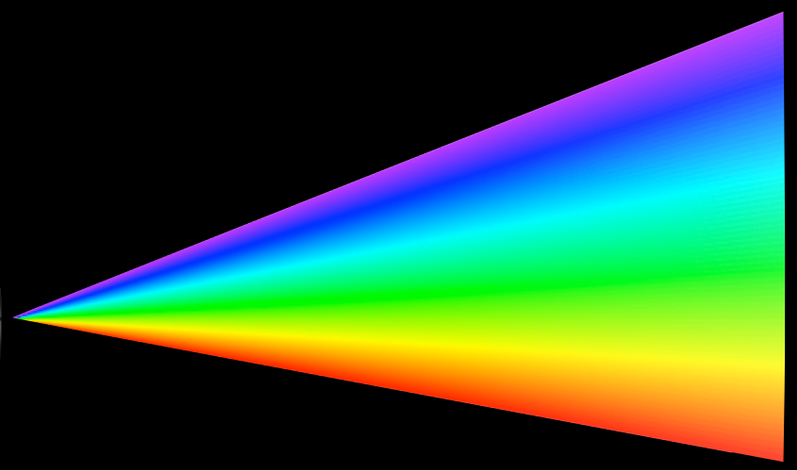
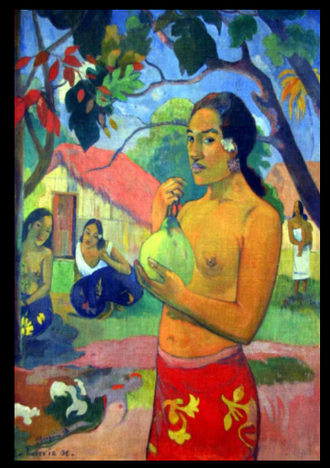




what color is all about







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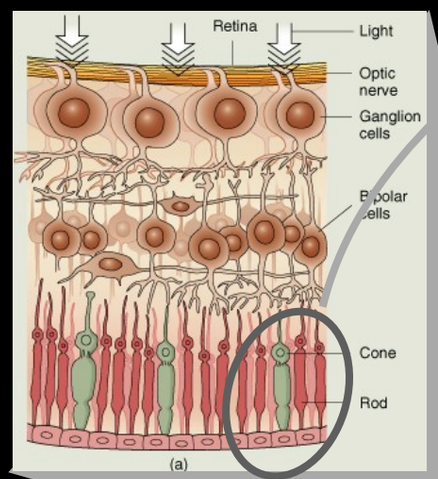
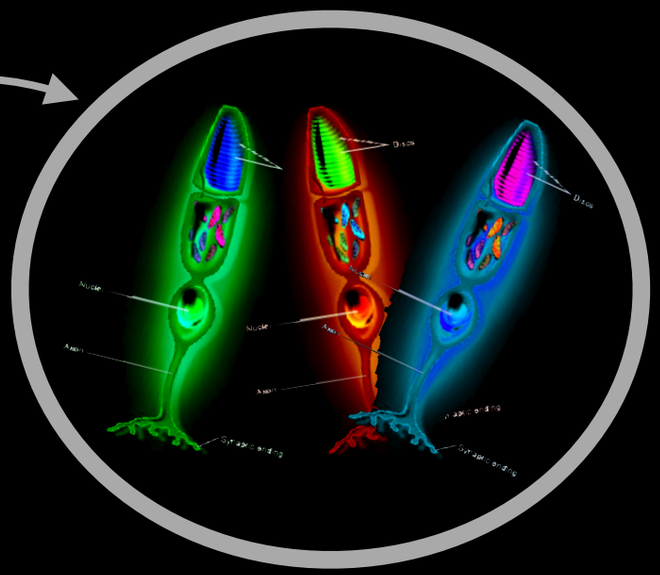
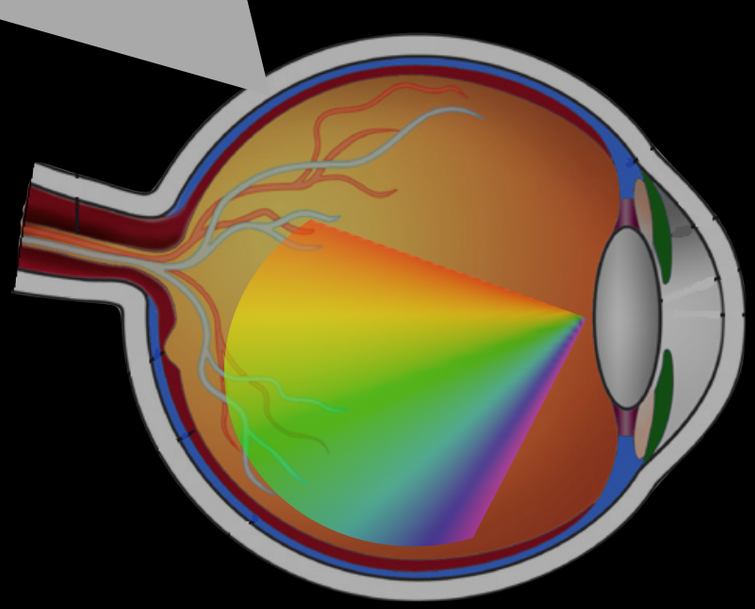
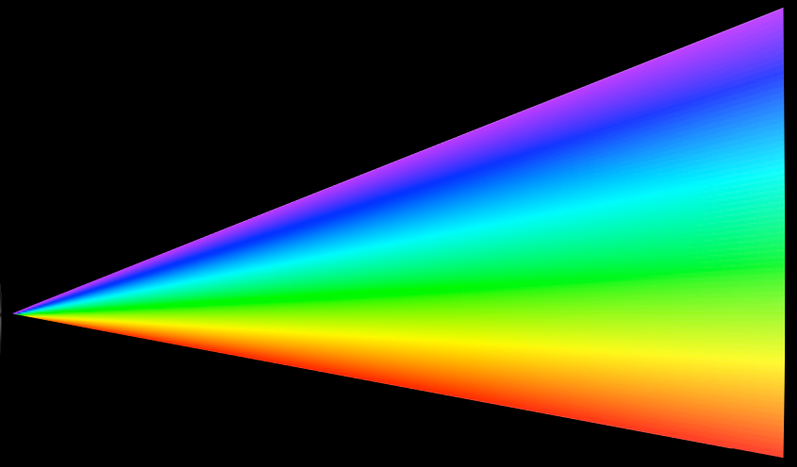
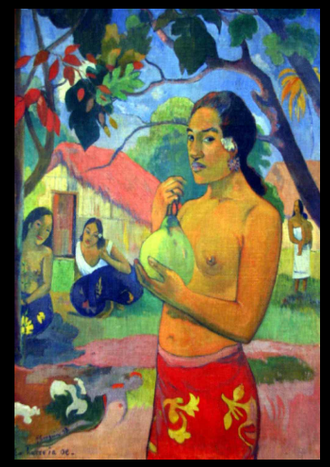


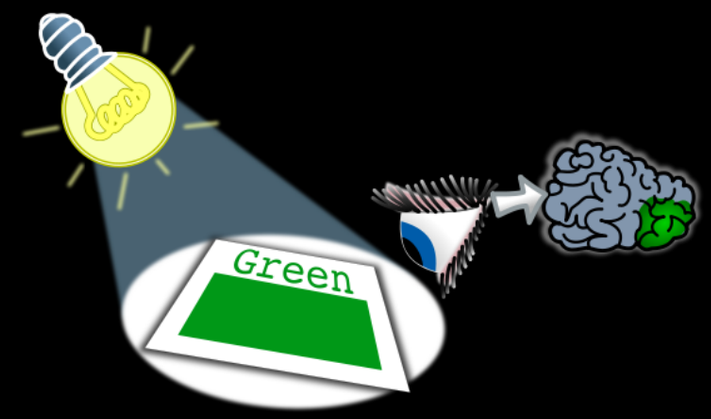






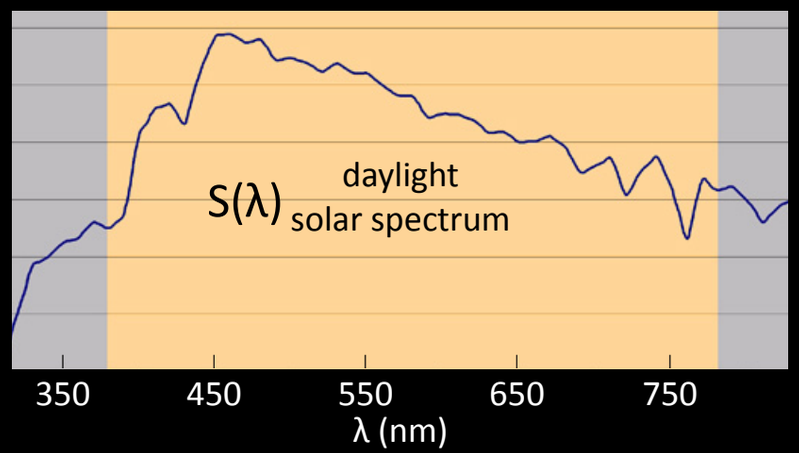


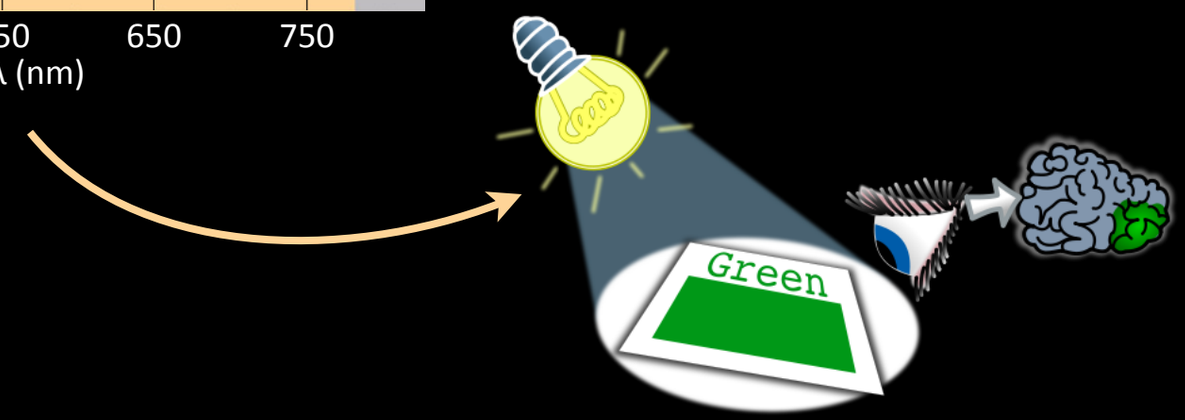
what color is all about



stimulus =
illuminant × transmission × sensitivity

what color is all about





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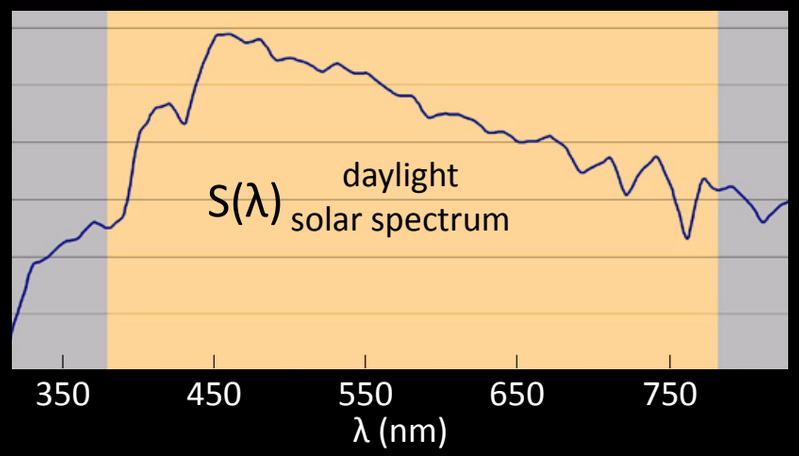

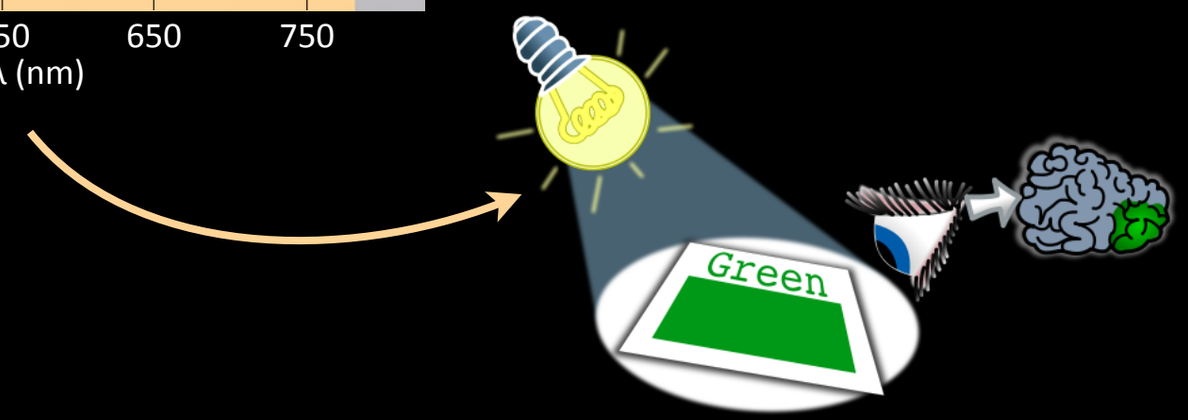

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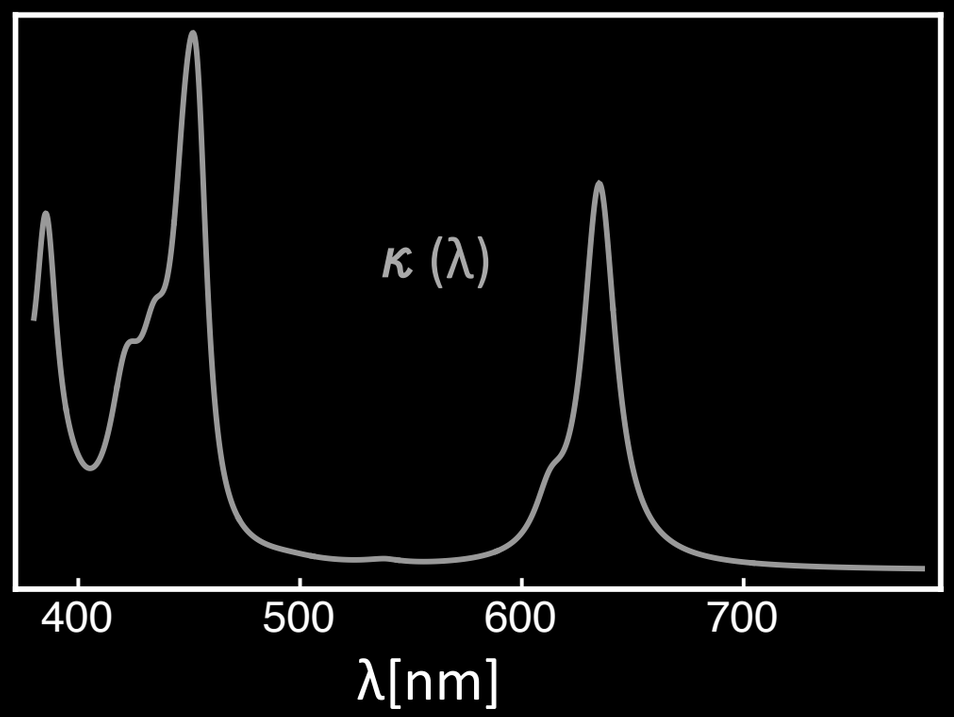

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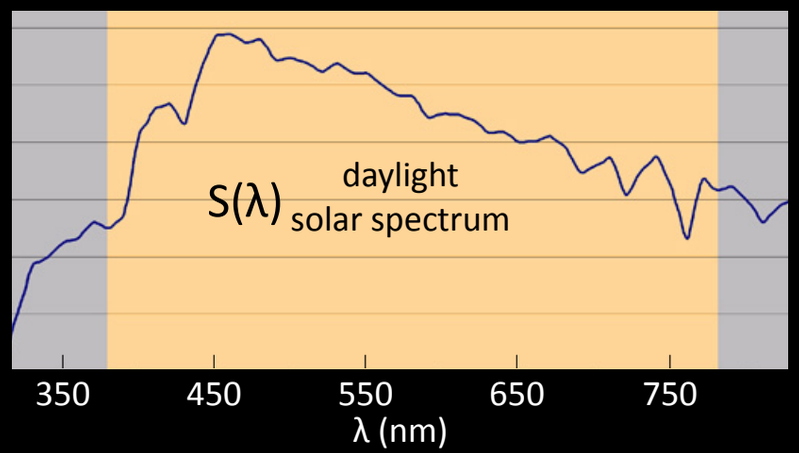

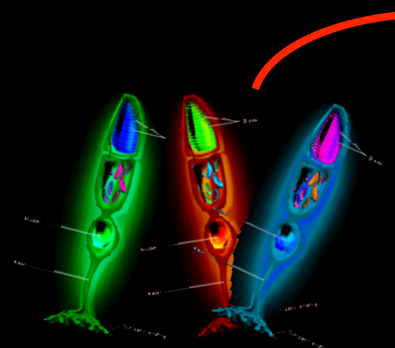

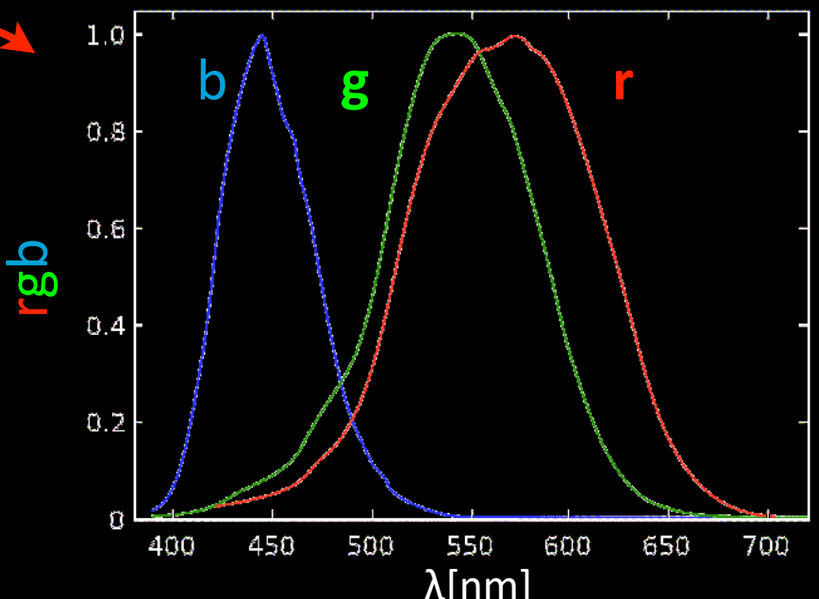

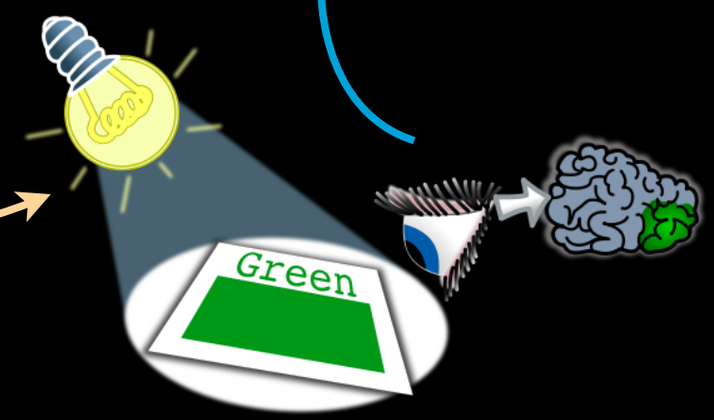

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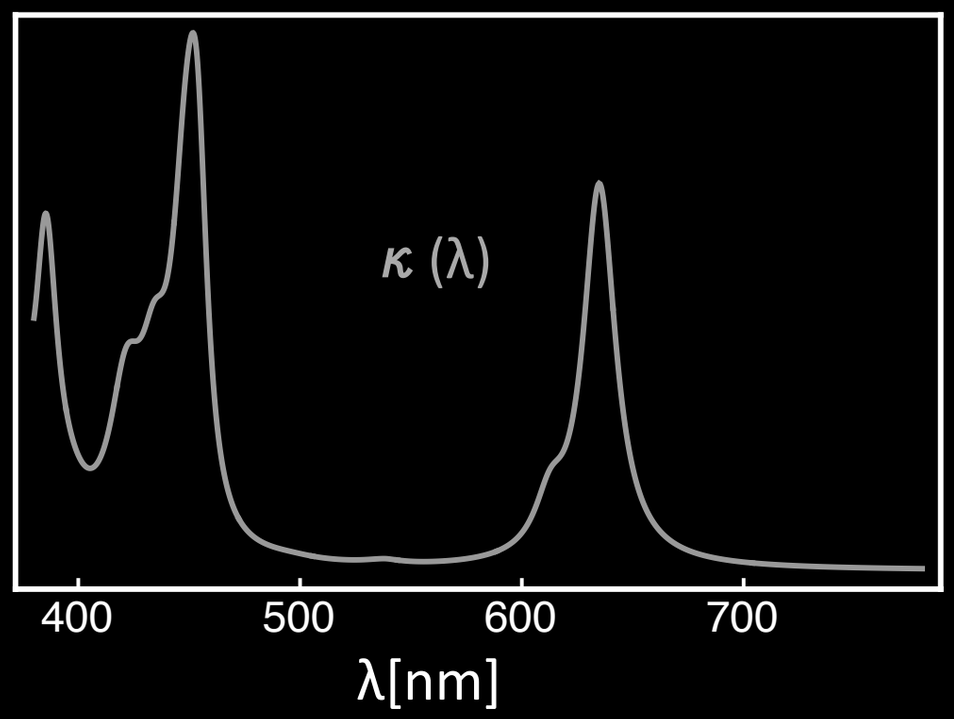

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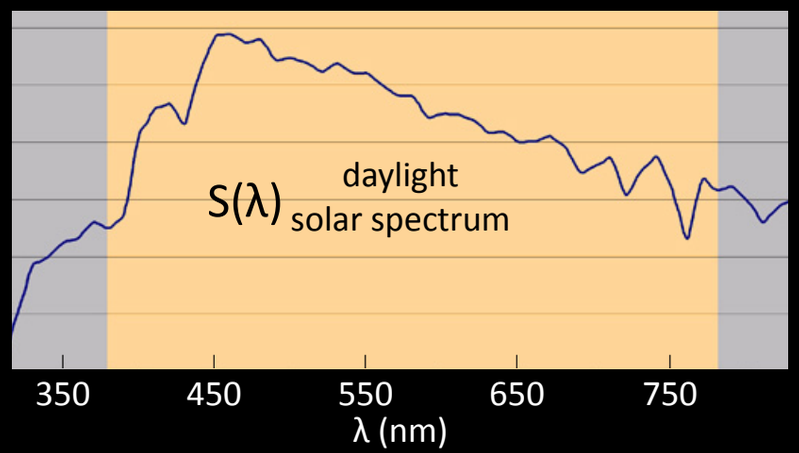

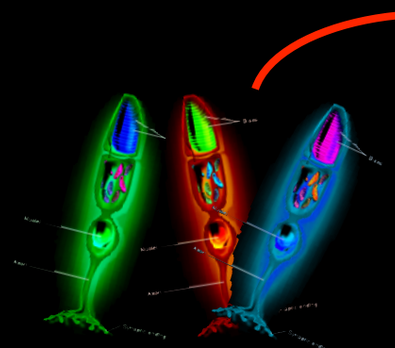

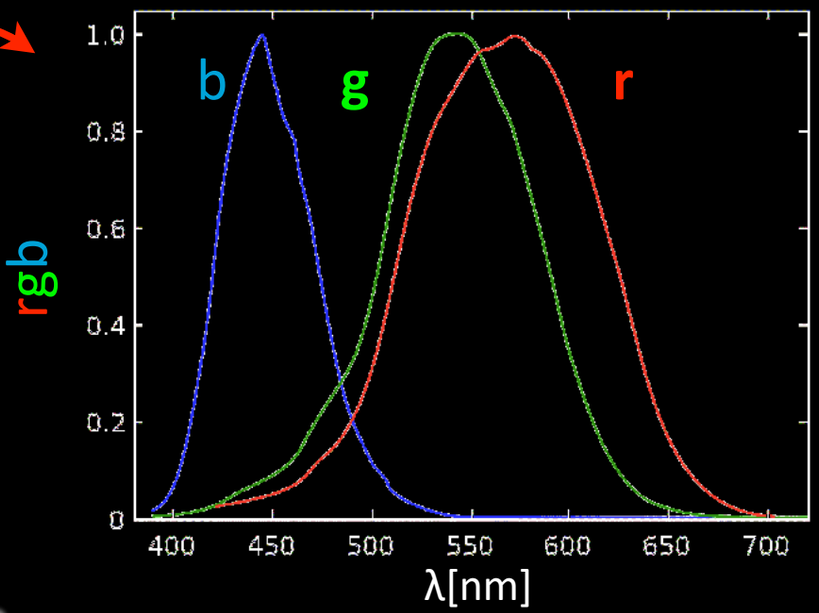

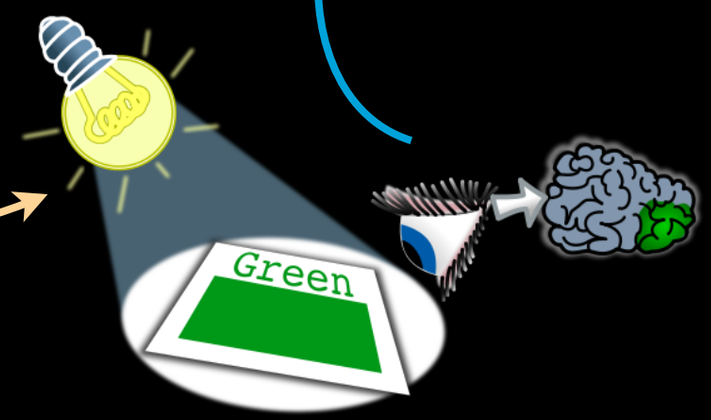

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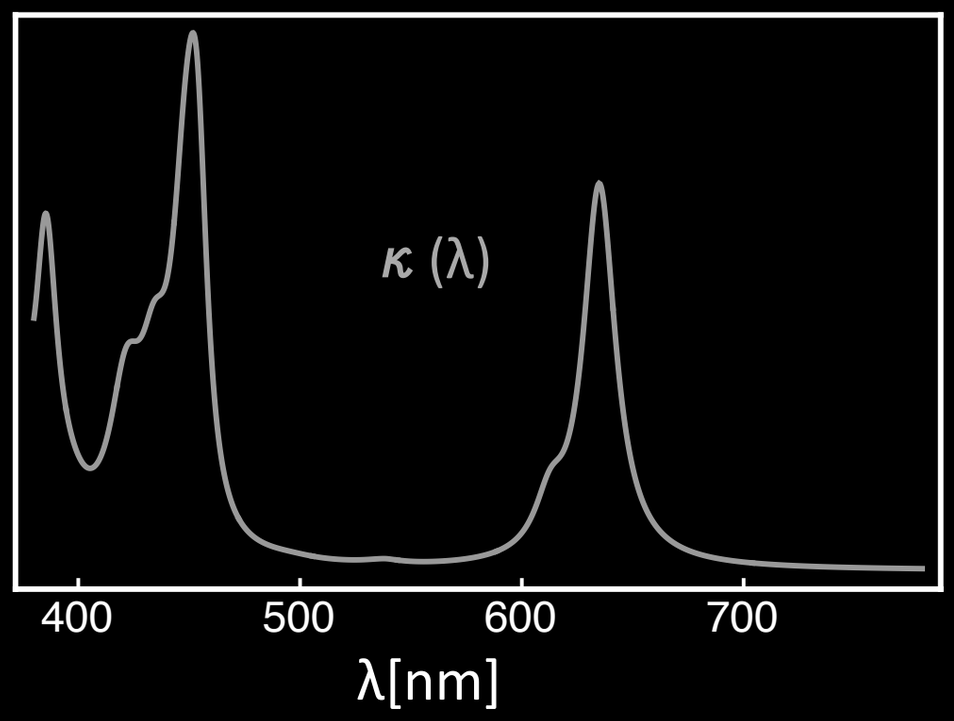
$$\mathrm{RGB}(x) = \int \mathrm{S}(\lambda)\mathrm{e}^{-\kappa(\lambda)x}\mathrm{rgb}(\lambda)d\lambda$$



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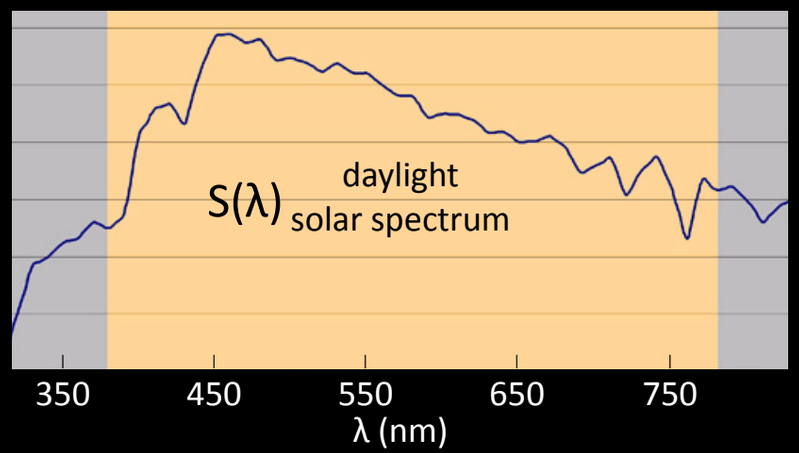

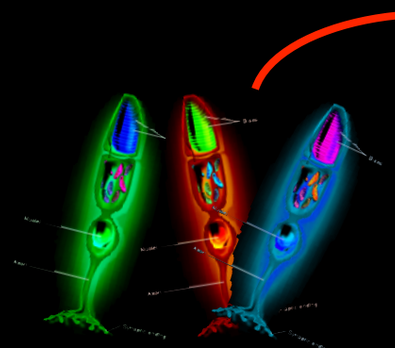

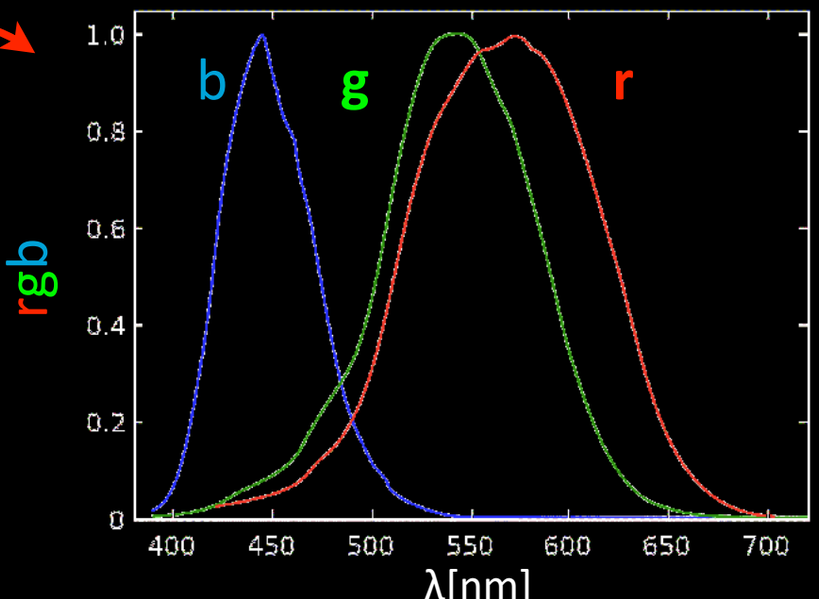

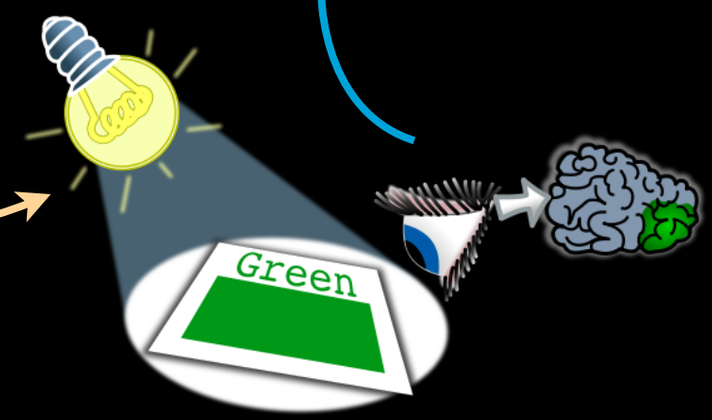

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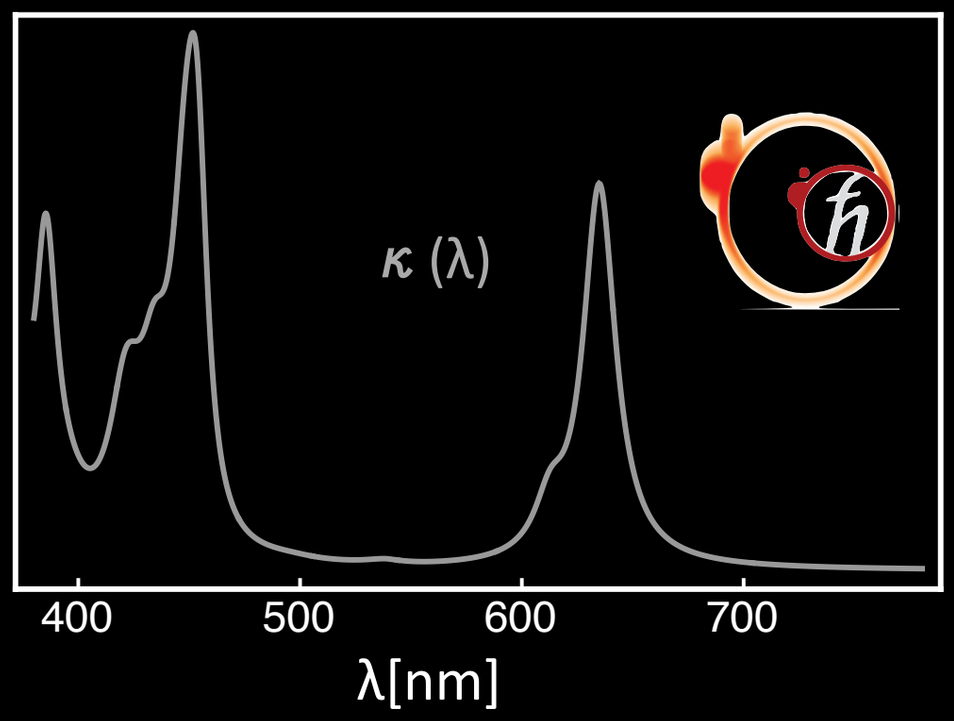
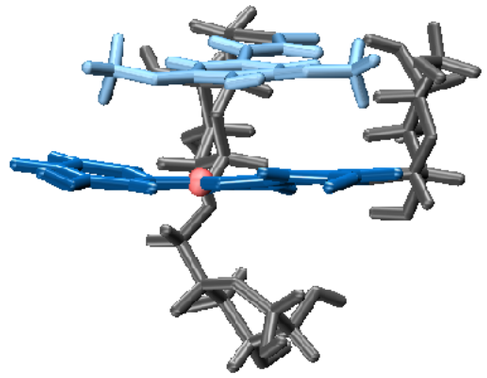


from chemistry to colour

chemical composition → molecular structure



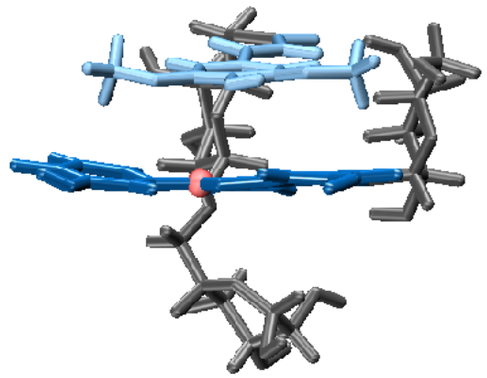
from chemistry to colour

chemical composition

+

environmental conditions

molecular structure



from chemistry to colour

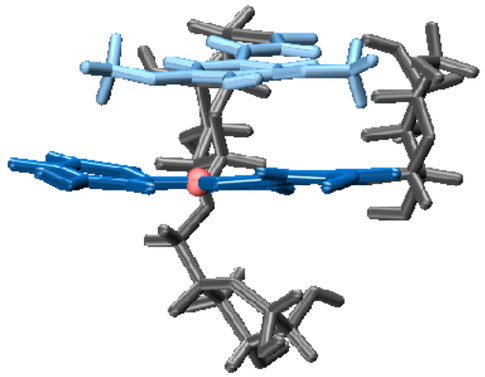
chemical composition

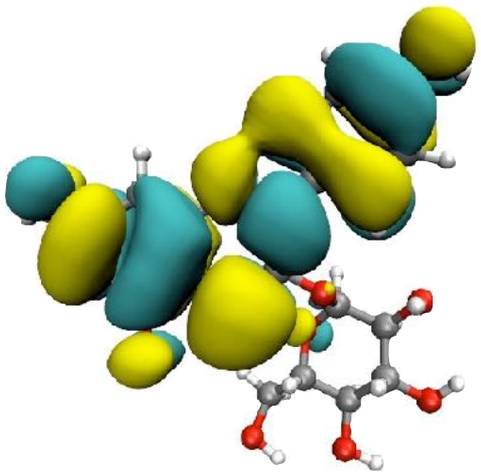
+

environmental conditions

molecular structure

electronic structure





from chemistry to colour

chemical composition

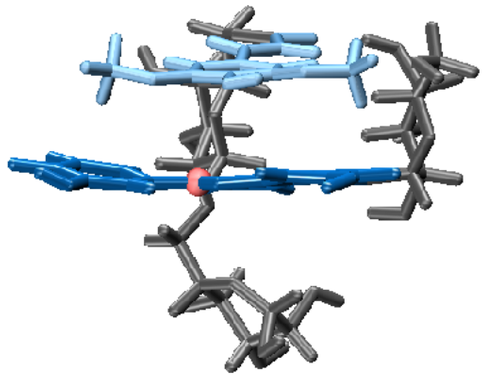
+

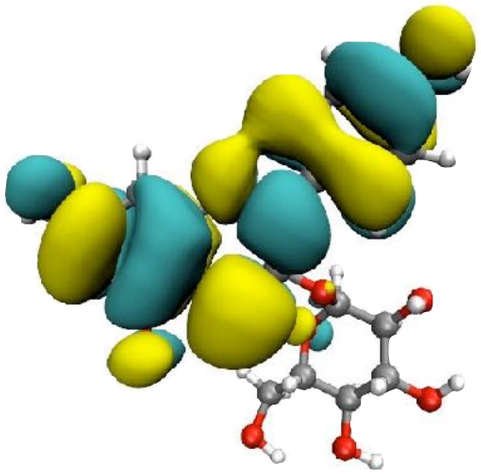
environmental conditions

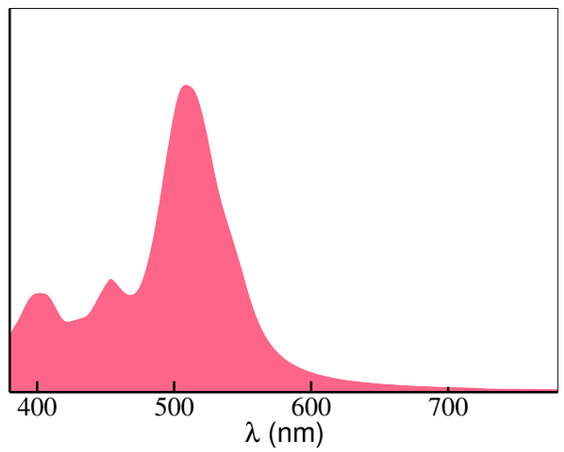
molecular structure

electronic structure

absorption spectrum







from chemistry to colour

chemical composition

+

environmental conditions

=

color

molecular structure

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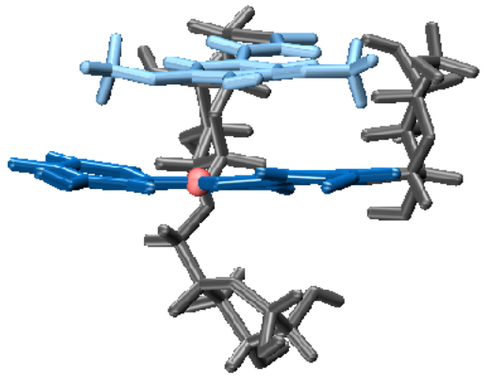
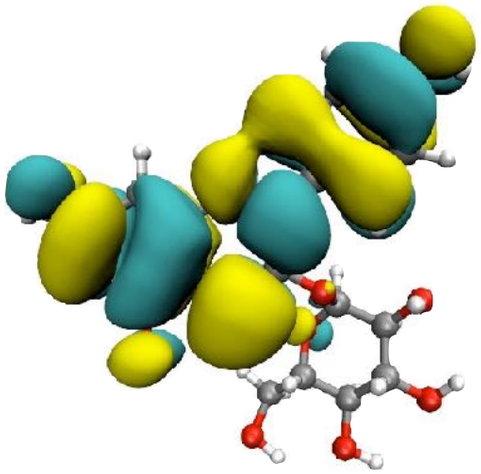
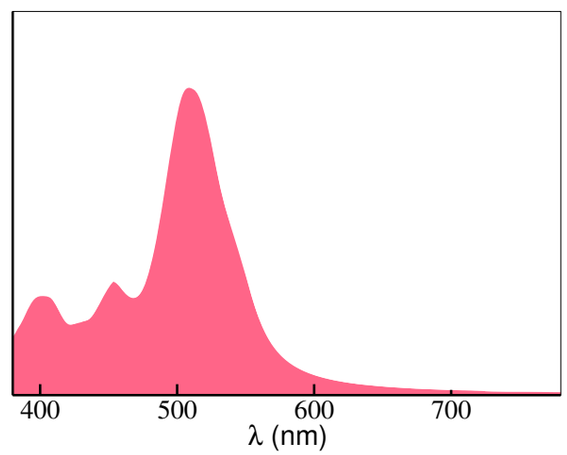
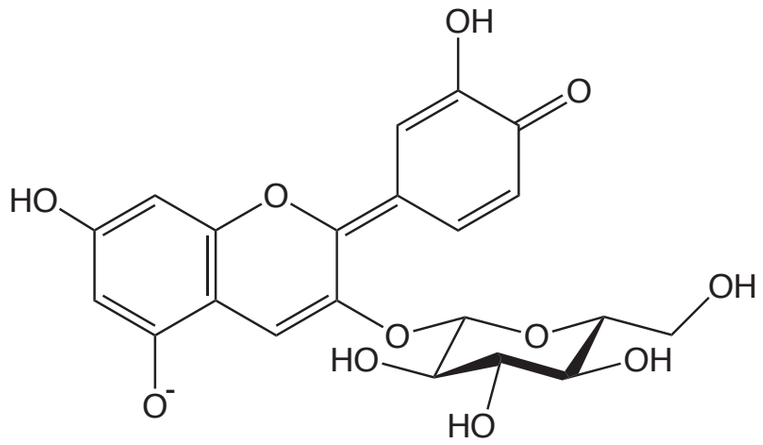
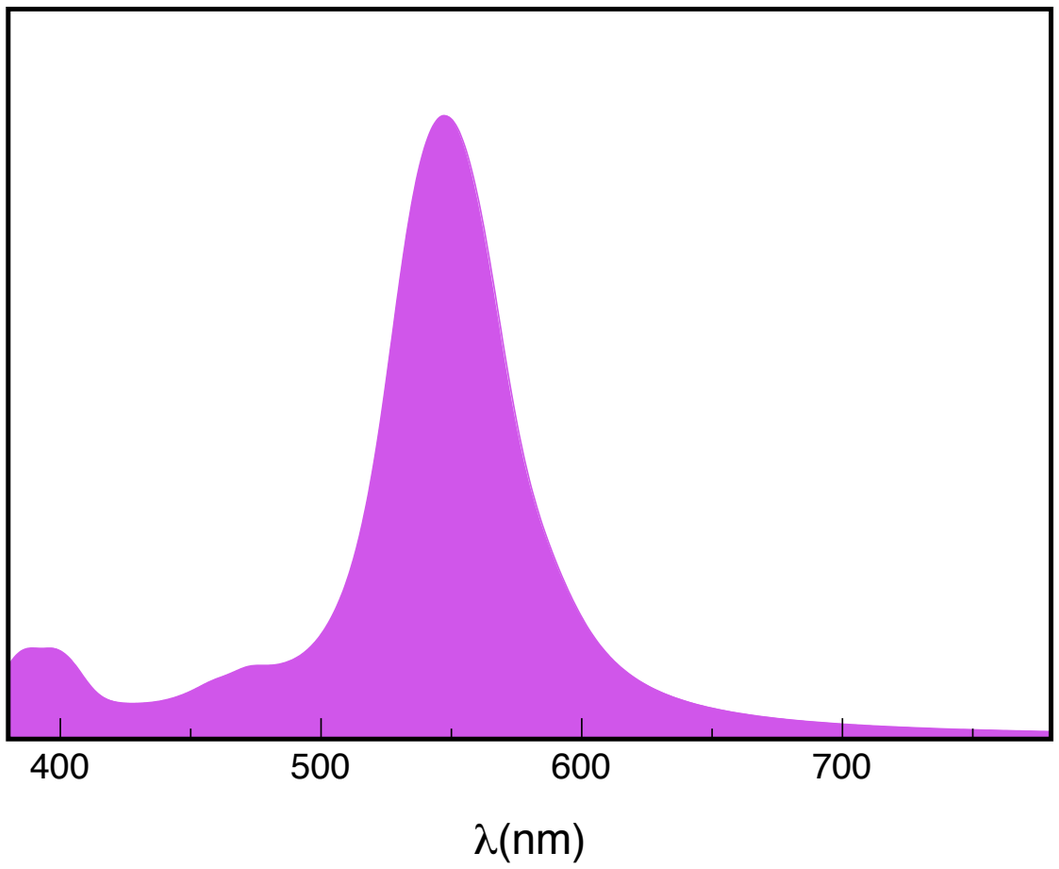




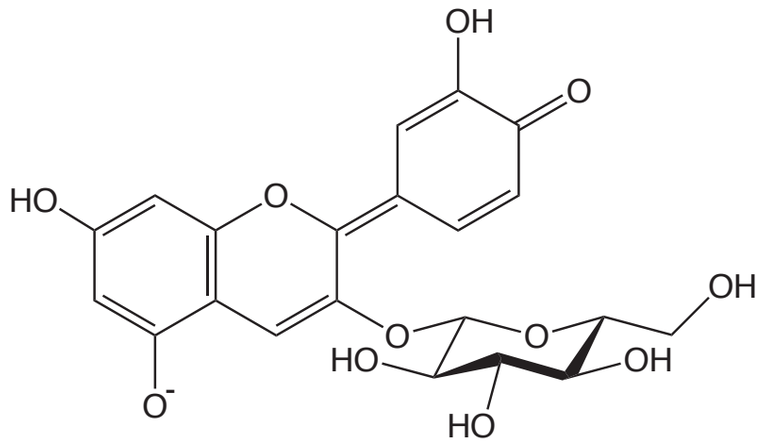


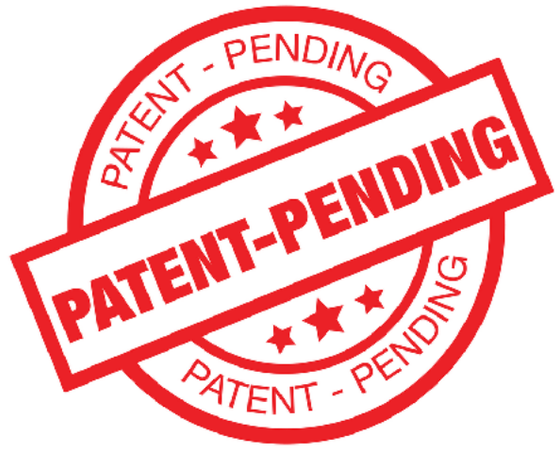
a newly identified substitute for “blue 2”

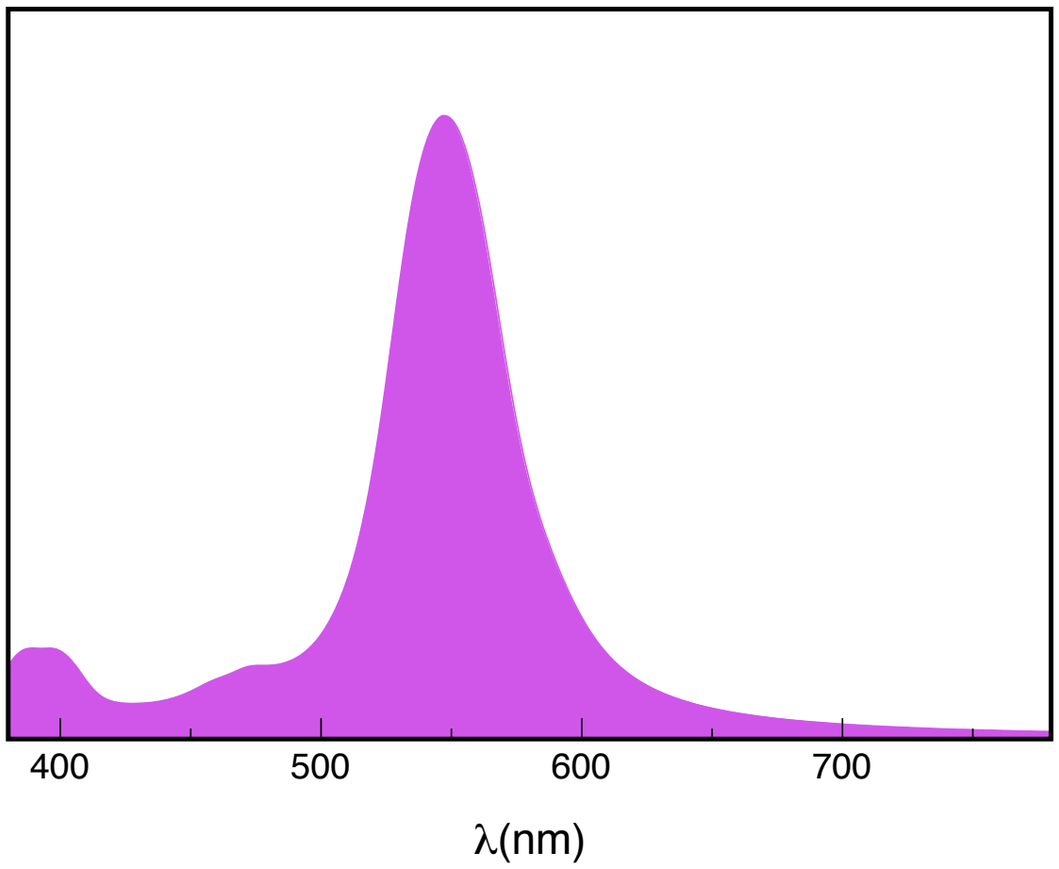


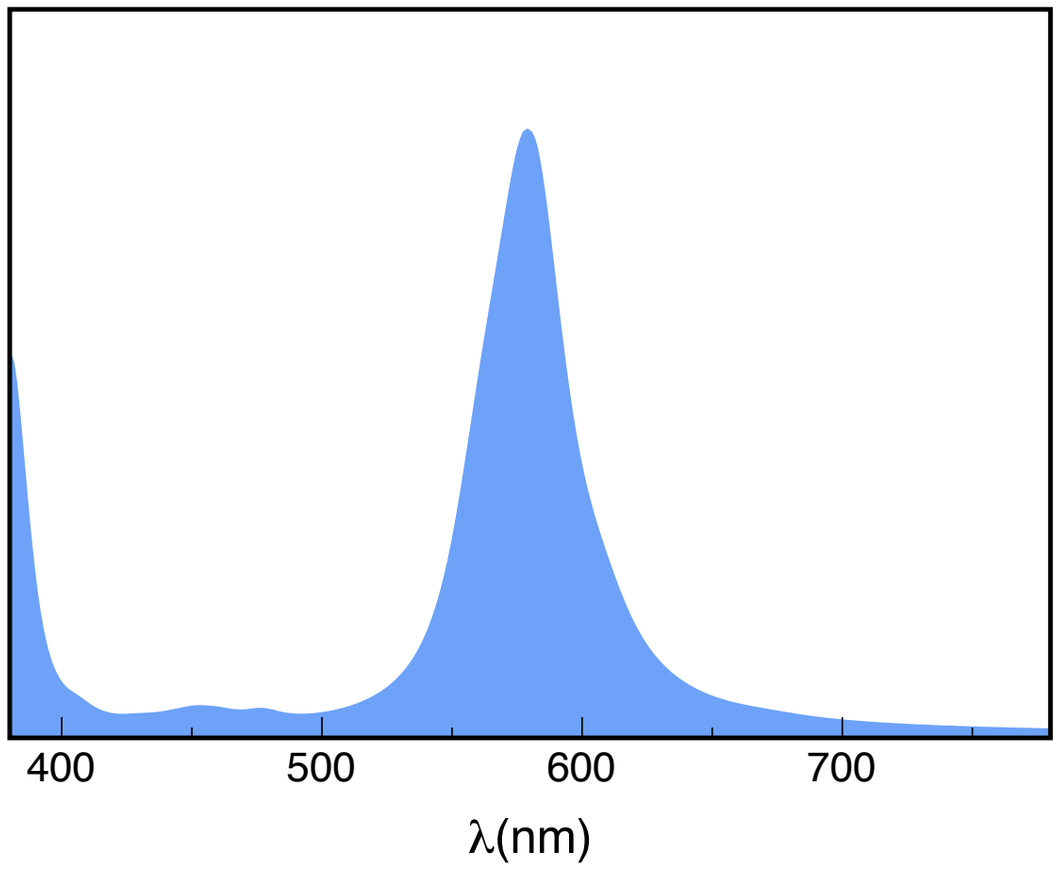


a newly identified substitute for “blue 2”







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