Quantum Chemistry – a Matter of Life and Death

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Monday Enrichment Seminar
Hybrid Technology Hub

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Hylleraas

Forskningsrådet

Senter for fremragende forskning

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Atoms and molecules

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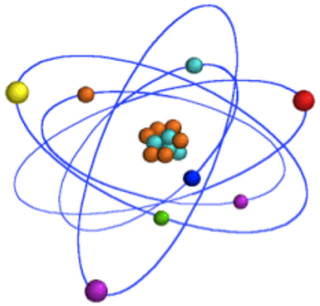
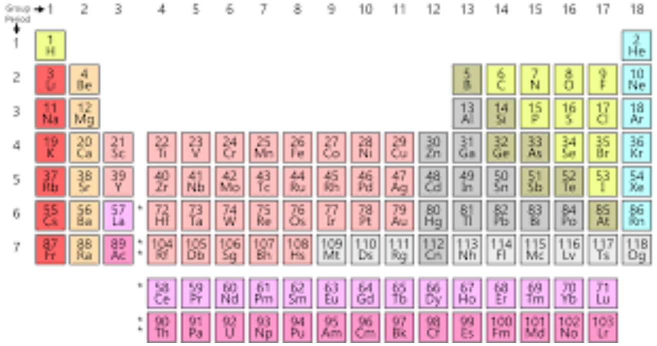
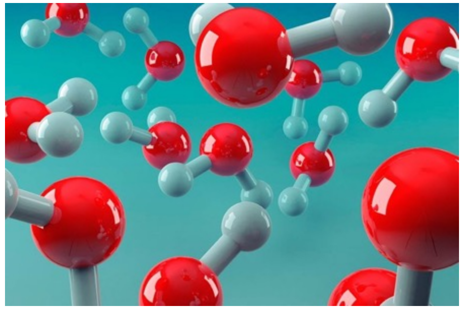
- Atoms are the building blocks of matter
  - a positively charged heavy nucleus
  - negatively charged light electrons

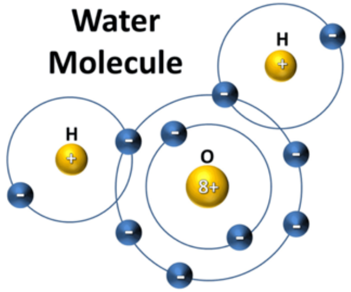




- When atoms attach to each other, we obtain molecules

H_2O





Molecules and quantum mechanics

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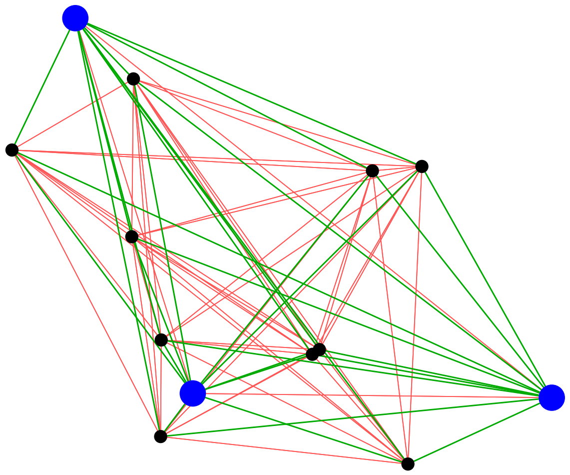
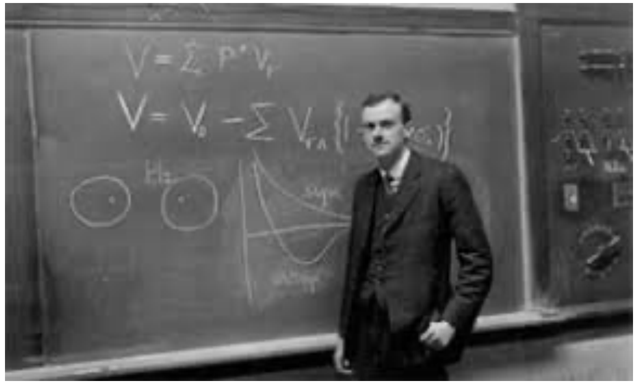
- Molecules are simple: charged particles in perpetual motion
  - nuclei repel one another
  - electrons repel one another
  - electrons and nuclei attract one another



- All particles obey the laws of quantum mechanics
  - we solve Schrödinger equation (1926) on computers
  - a complicated many-body problem

$$-i\frac{\partial}{\partial t}\Psi(x_1,\dots x_N,t) = \left(-\frac{1}{2}\sum_i \nabla_i^2 - \sum_{iI}\frac{Z_I}{r_{iI}} + \frac{1}{2}\sum_{i\neq j}\frac{1}{r_{ij}}\right)\Psi(x_1,\dots x_N,t)$$

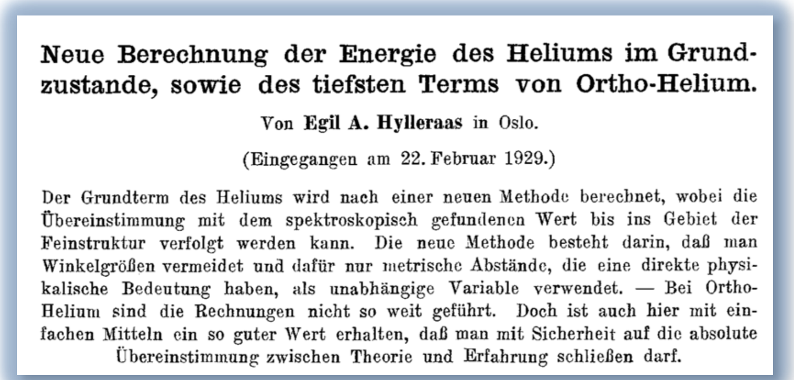


Paul Dirac (1929):

> 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. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed…

Egil Hylleraas (1898–1965)

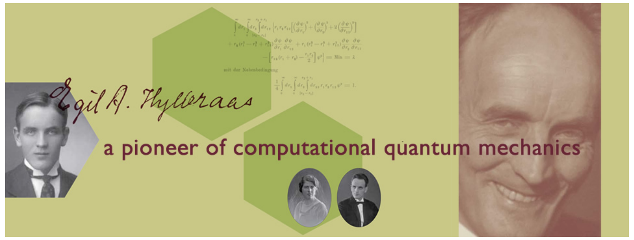
- established computational electronic-structure theory

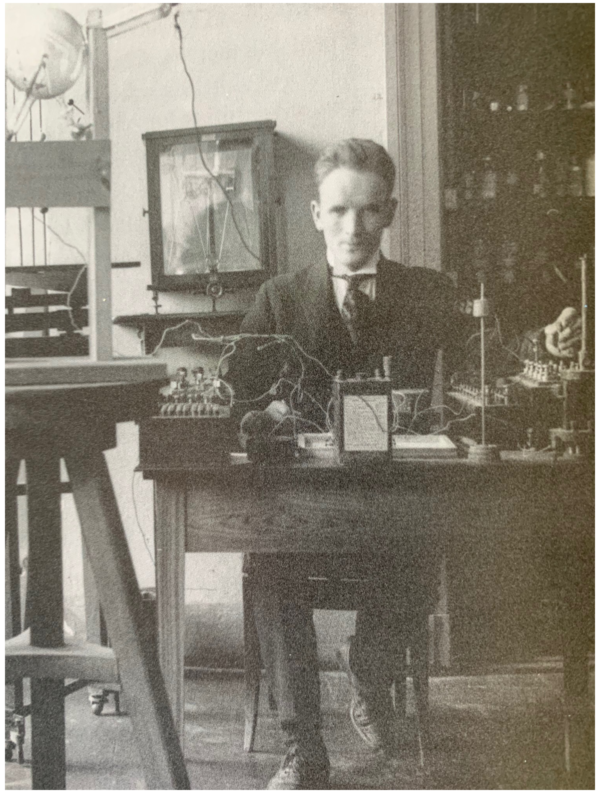

Neue Berechnung der Energie des Heliums im Grundzustande, sowie des tiefsten Terms von Ortho-Helium.

Von **Egil A. Hylleraas** in Oslo.

(Eingegangen am 22. Februar 1929.)

Der Grundterm des Heliums wird nach einer neuen Methode berechnet, wobei die Übereinstimmung mit dem spektroskopisch gefundenen Wert bis ins Gebiet der Feinstruktur verfolgt werden kann. Die neue Methode besteht darin, daß man Winkelgrößen vermeidet und dafür nur metrische Abstände, die eine direkte physikalische Bedeutung haben, als unabhängige Variable verwendet. — Bei Ortho-Helium sind die Rechnungen nicht so weit geführt. Doch ist auch hier mit einfachen Mitteln ein so guter Wert erhalten, daß man mit Sicherheit auf die absolute Übereinstimmung zwischen Theorie und Erfahrung schließen darf.





Help came from unexpected quarters...

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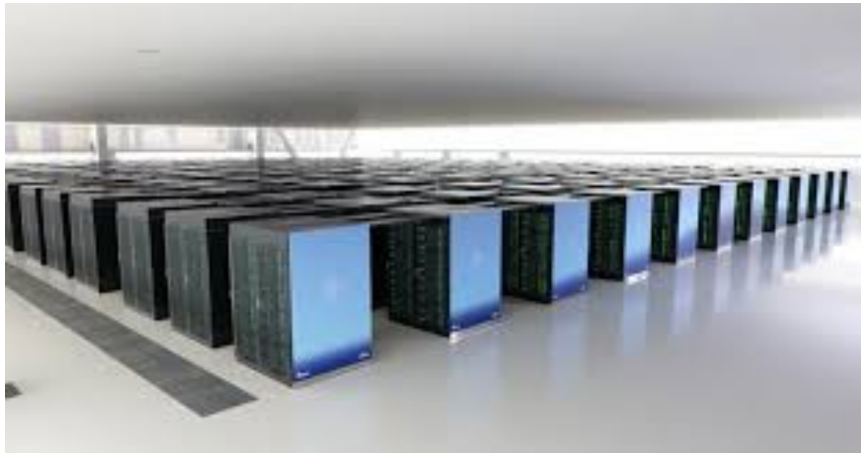
- Eniac (1948) 0.5 kFLOPS ≈ 10^3
- Cray 2 (1985) 1.9 GFLOPS ≈ 10^9
- Fugaku (2020) 0.4 EFLOPS ≈ 10^{18}



From simple to complex systems

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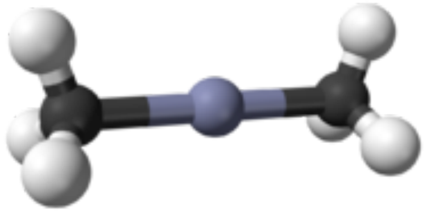
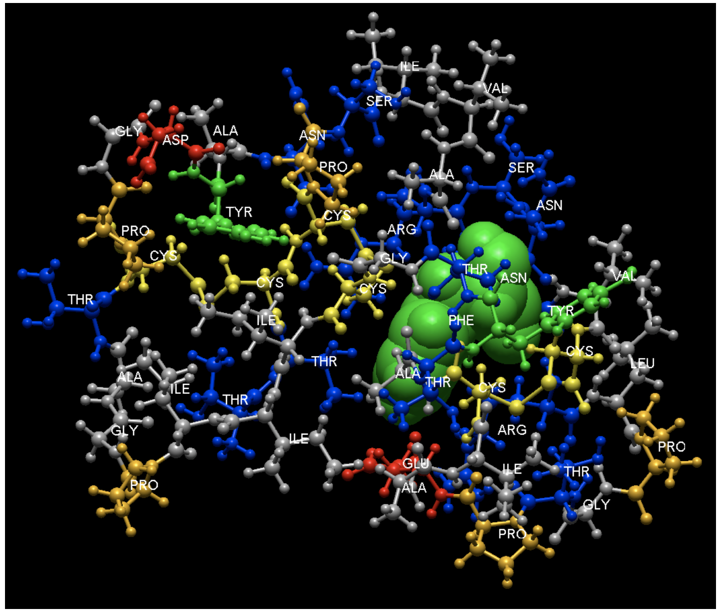
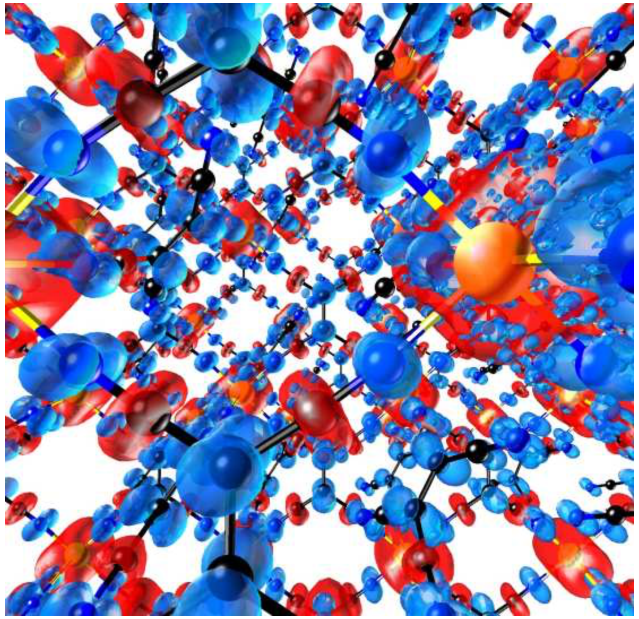
- Forty years ago we studied small molecules
  - of limited interest and impact
- Today we are studying hundreds of atoms
  - biological systems and materials







Simulation — the third way of science

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- Experiments, theory — and simulation
  - interpretation and prediction of experiments
  - alternative to (difficult, expensive or dangerous) experiments
- Every third CoE makes heavy use of simulations
  - Hylleraas Centre consumes about 40 MCPU hours annually

BJERKNES CENTRE for Climate Research

CMA Centre of Mathematics for Applications

Center for Biomedical Computing

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CEED

Rosseland Centre for Solar Physics

Kavli Institute for Systems Neuroscience
Centre for Neural Computation

QuSpin

CTCC The Centre for Theoretical and Computational Chemistry

cbd CENTRE FOR BIODIVERSITY DYNAMICS

PoreLab NTNU-UiO Porous Media Laboratory

PGP PHYSICS OF GEOLOGICAL PROCESSES

Mathematics and chemistry

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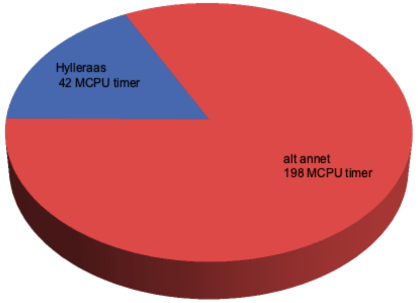
Every attempt to employ mathematical methods in the study of chemical questions must be considered profoundly irrational. If mathematical analysis should ever hold a prominent place in chemistry—an aberration which is happily impossible—it would occasion a rapid and widespread degradation of that science.

August Comte (1798–1857)

The more progress sciences make, the more they tend to enter the domain of mathematics, which is a kind of centre to which they all converge. We may even judge the degree of perfection to which a science has arrived by the facility with which it may be submitted to calculation.



Adolphe Quetelet (1796– 1874)

Electron density — electron cloud

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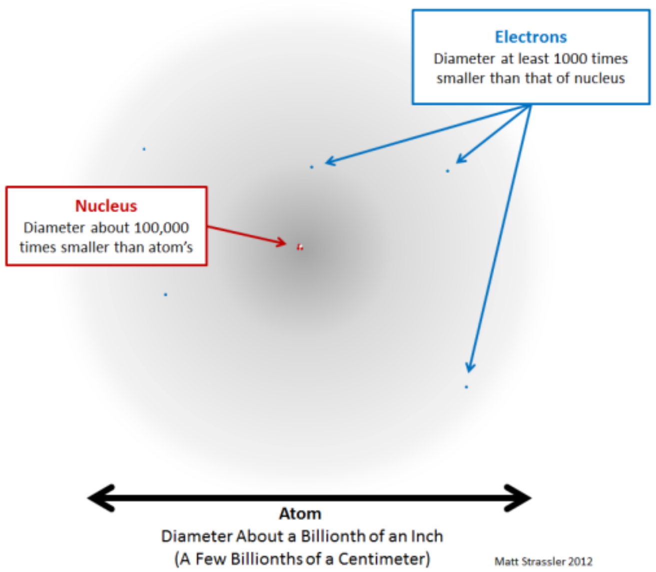
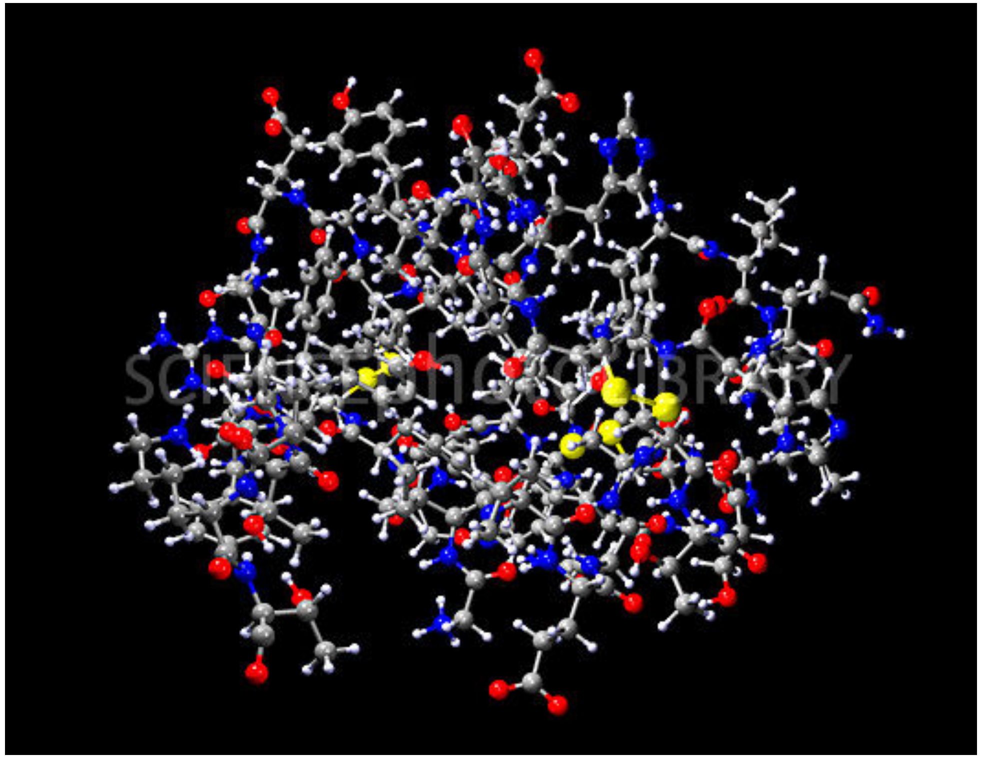
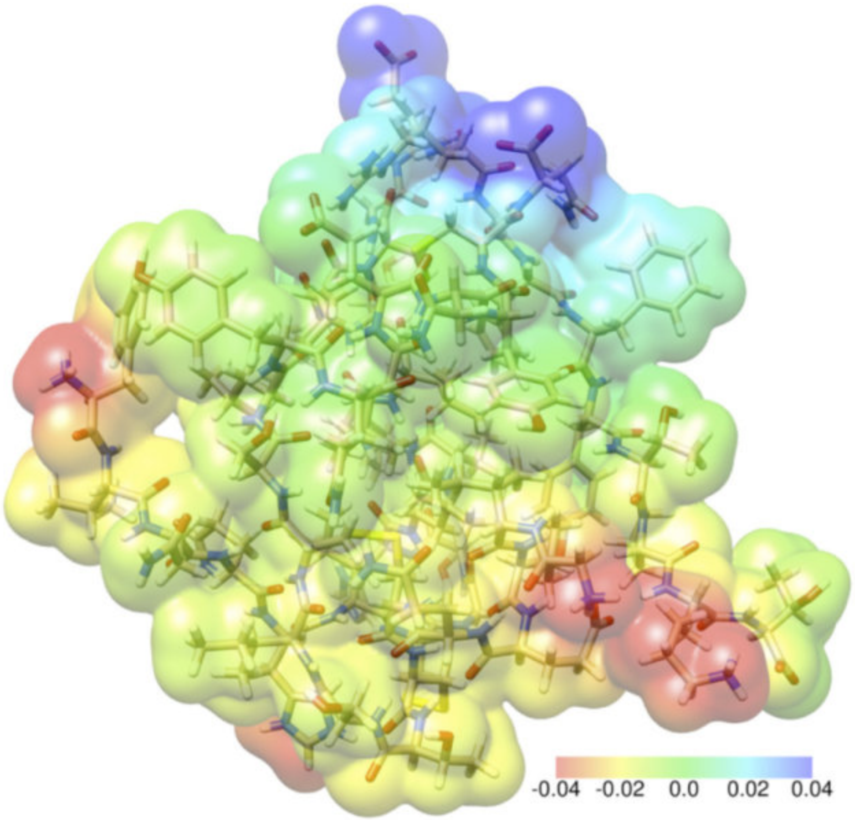
- Electrons live an ephemeral, fleeting existence — constantly on the run
  - they are nowhere before we find them— then they disappear again
- We calculate the probability for finding them at each point in space
  - this probability is the electron density or electron cloud (Max Born 1926)



Insulin molecule and its density

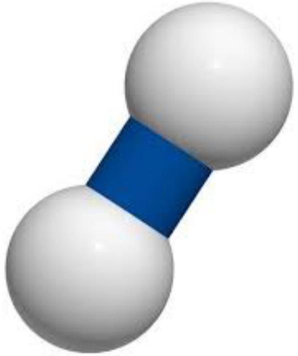


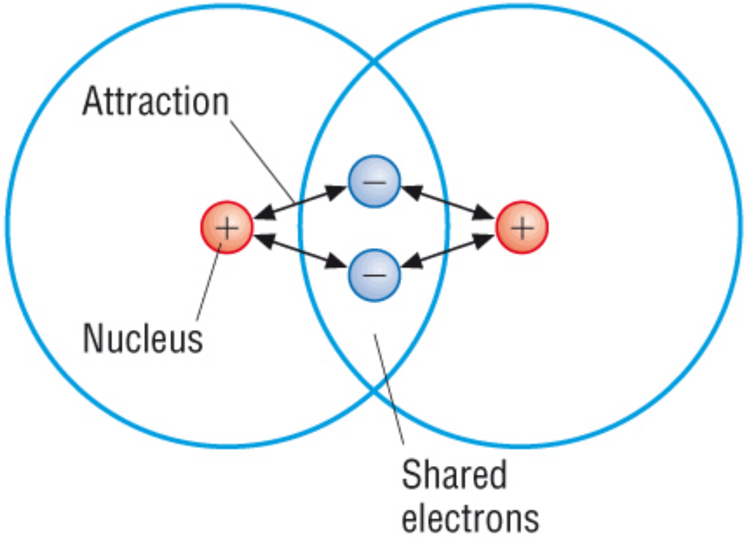


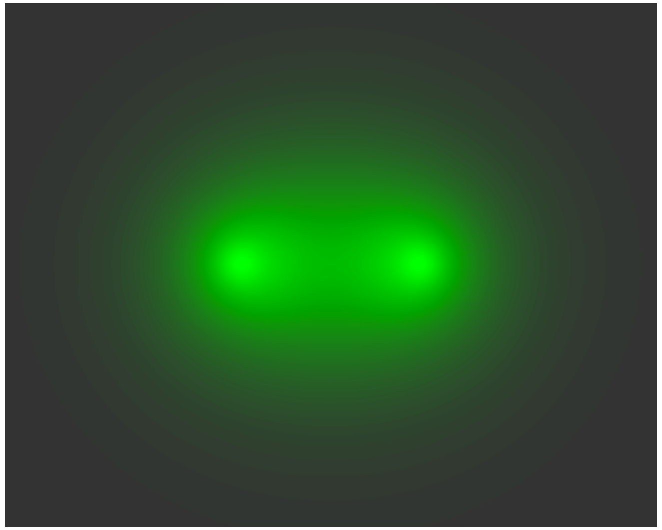
787 nuclei + 3106 electrons = 3893 particles

Chemical bond

- Molecules are formed when atoms bind to each other
  - the simplest molecule is the hydrogen molecule: H_2
  - each atom contributes one electron
  - the electrons are most often found between the nuclei
- Covalent bond — can be understood electrostatically

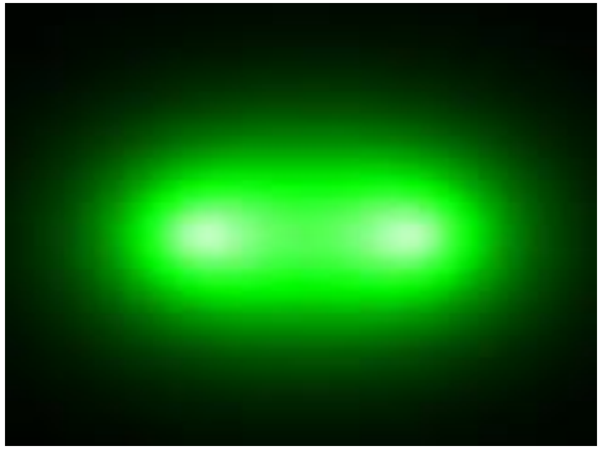


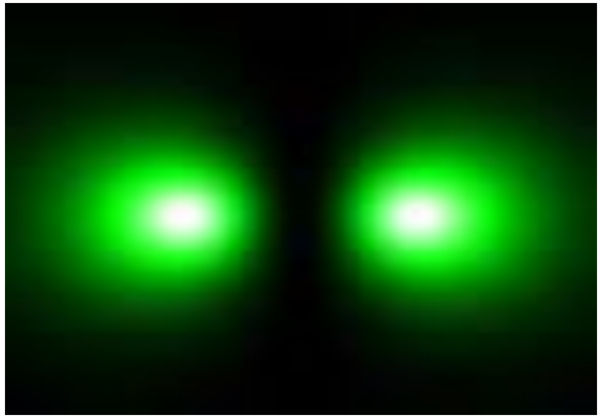




Quantum states

- Atoms and molecules exist in different quantum states
  – each state has a specific energy and density
- The two lowest states of the hydrogen molecule H_2
  – two nuclei and two electrons
- In the ground state H_2 has its lowest energy and is bound
  – accumulation of electrons between the nuclei
- In the first excited state H_2 is not bound
  – depletion of electrons between the nuclei





Quantum leaps

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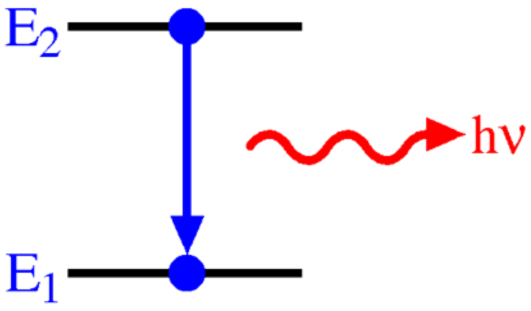
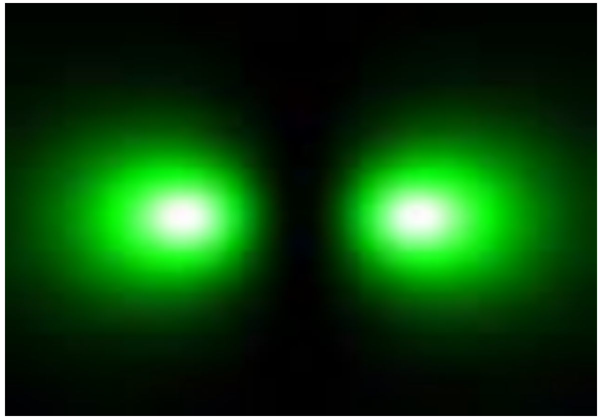
- The energy of a molecule is quantized
  - only energy levels that correspond to quantum state are allowed
- A molecule can perform quantum leaps between levels
  - instantaneous and total change of the state with no warning
- How is energy conserved?
  - typically by emitting or absorbing a photon — particle of light





Radiation and photons

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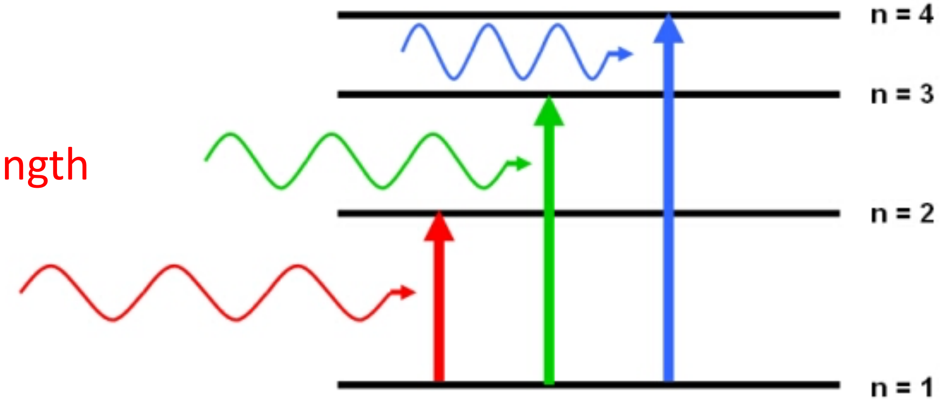
- Radiation is a stream of particles called photons
  - photons have no mass and travel at the speed of light
  - each photon has an energy inversely proportional to the wave length

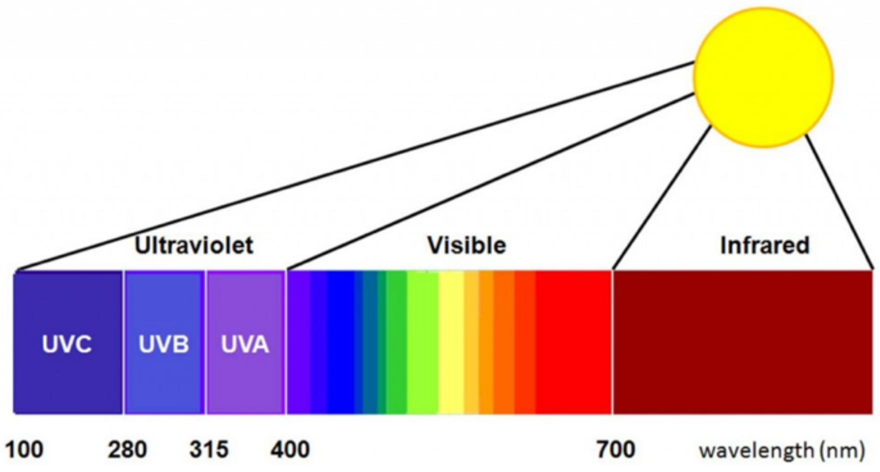
$$E = \frac{hc}{\lambda}$$



  - photons may be absorbed or emitted if they have the right energy

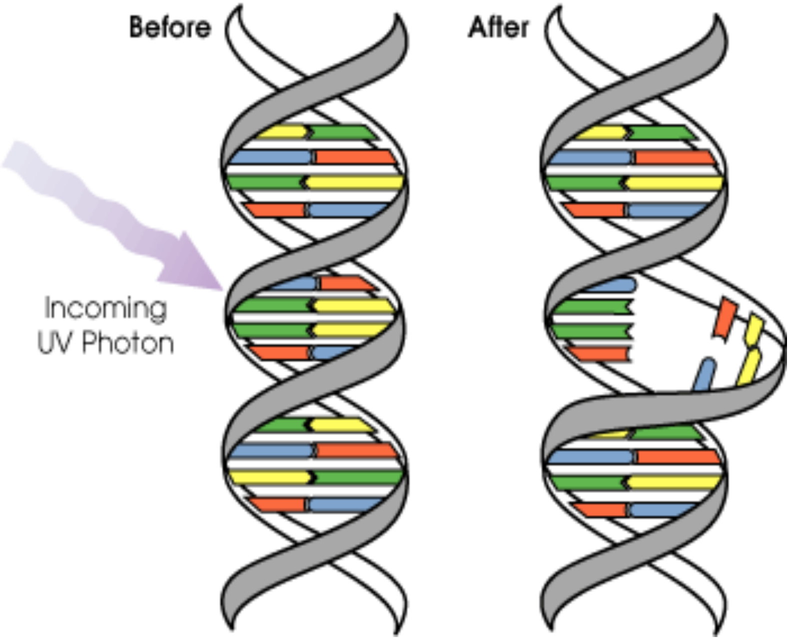
- The Sun emits mostly visible photons
  - 10^{16} photons hit the eye every second in daylight

- The Sun emits also non-visible photons
  - ultraviolet photons have more energy than visible photons
  - infrared photons have less energy than visible photons



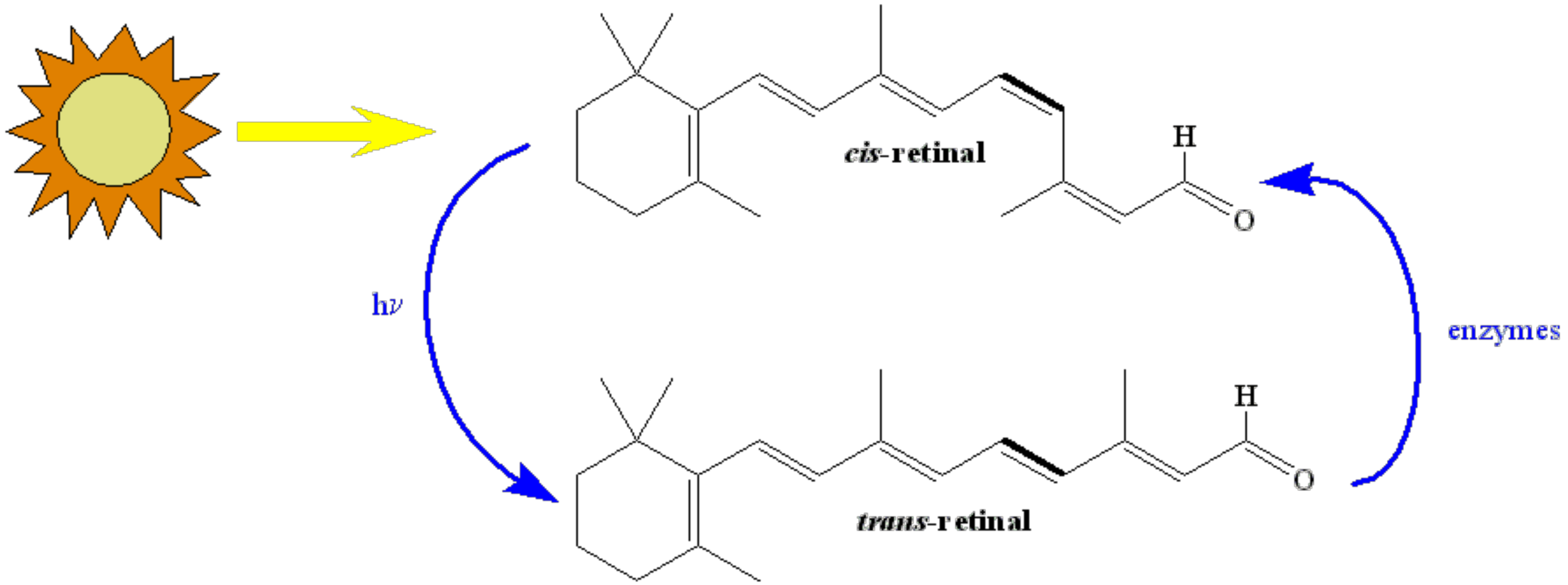
Ultraviolet photons

- UV photons can excite electrons from binding to antibinding state
  - UV photons may therefore break bonds and damage or destroy molecules
  - UV photons from the Sun can damage DNA moleucle (most often repaired)
  - visible and infrared photons have too little energy to break bonds



Visible photons

- A visible photon does not have sufficient energy to break bonds but may twist them
- In the human eye, a visible photon triggers cis- to trans- isomerization of retinal
  - the energy from the photon is then transformed to a nerve signal to the brain
  - an enzyme helps retinal regain its original cis form



Infrared photons

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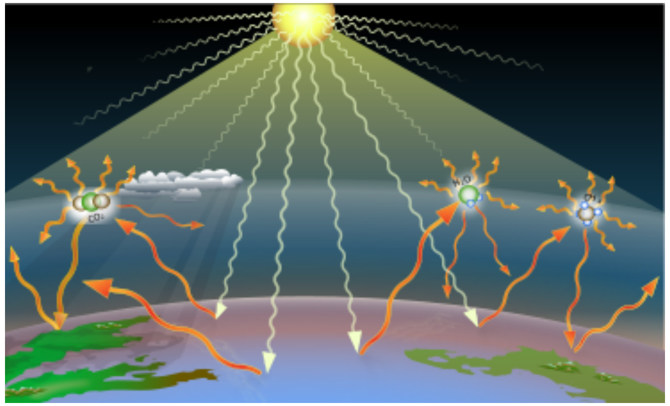
- Infrared photons have less energy the visible photons
  - they cannot twist retinal
  - they do not generate nerve signals

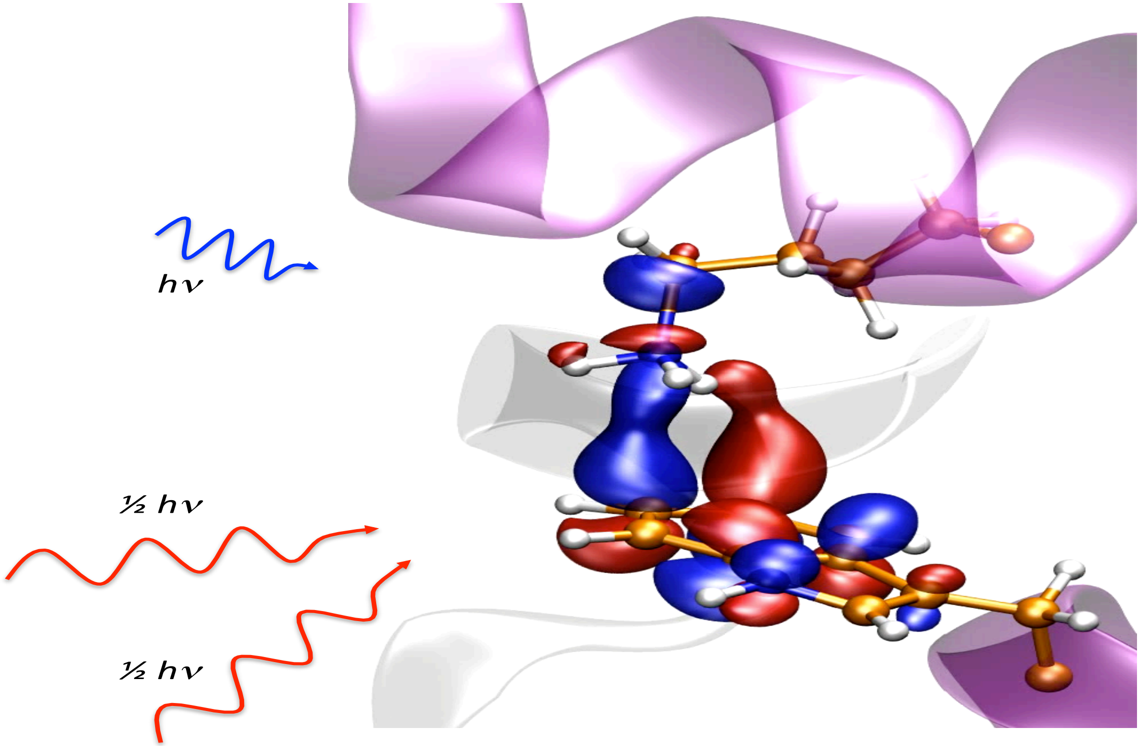


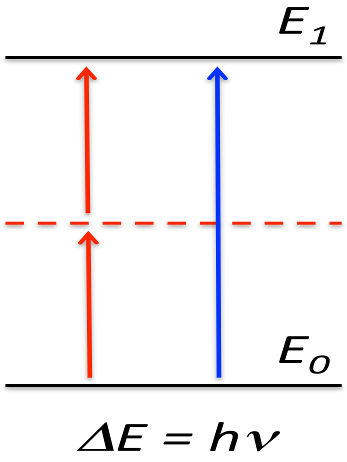
- Infrared photons induce molecular vibrations
  - we experience this as heat — thermal radiation
  - green house effect by absorption of infrared photons
  - infrared photons generate images in infrared cameras

- BUT: humans may see infrared radiation
  - radiation must be sufficiently intense
  - infrared radiation is seen as green light

Infrared vision

- Two infrared photons have the same energy a single visible photon
  - at sufficiently high photon density, retinal may absorb two photons at the same time
  - we showed how this is possible by performing advanced quantum-chemical calculations





Two-photon absorption (TPA)

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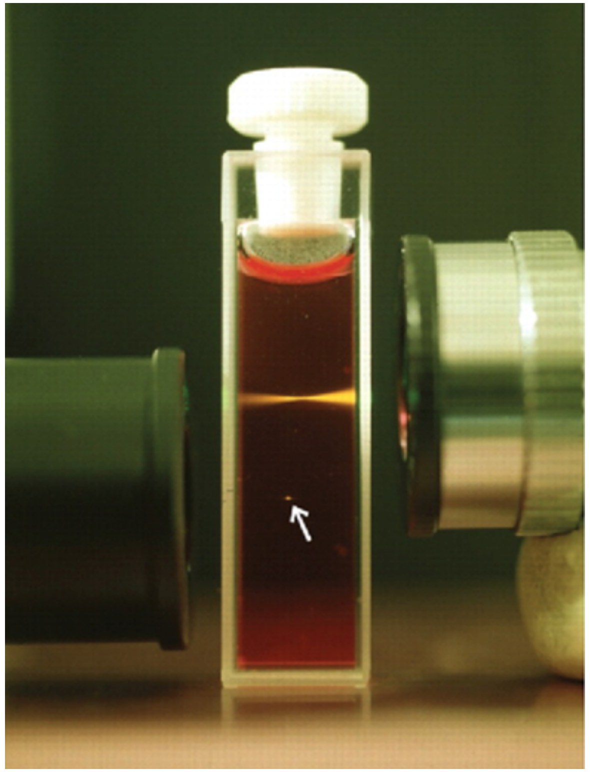
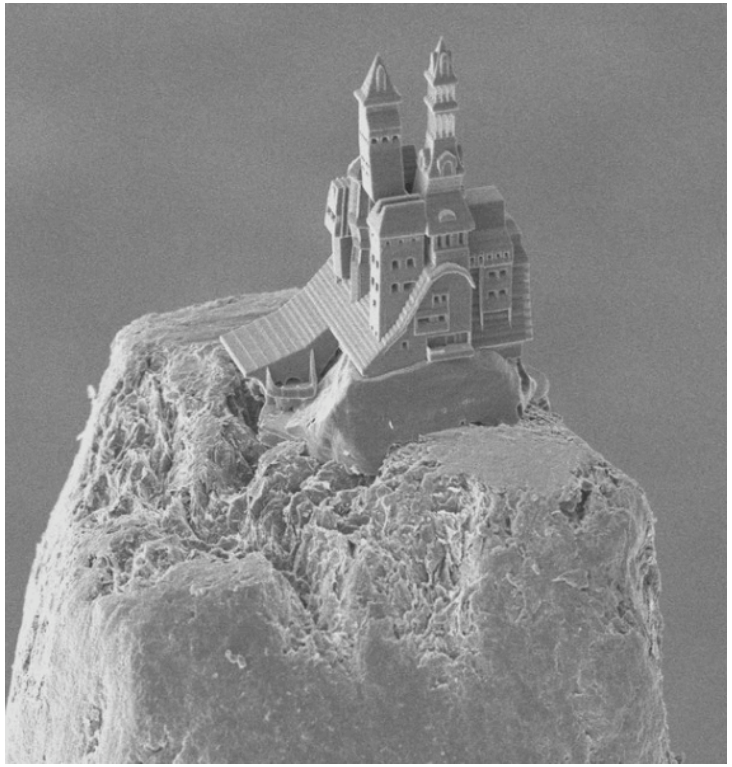
- Many exciting applications of two-photon absorption
  - two-photon absorption occurs only in a focus region — one-photon processes occur everywhere
  - medical imaging, photodynamic therapy, lithography, optical data storage





Cold adaptation of enzymes

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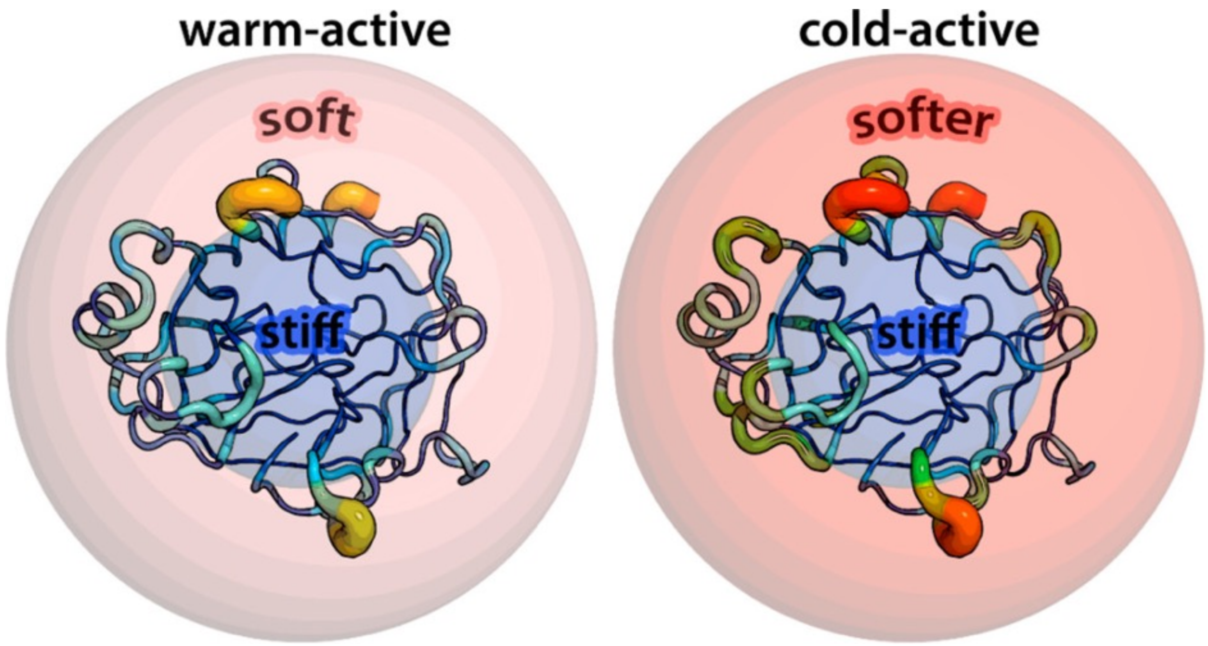
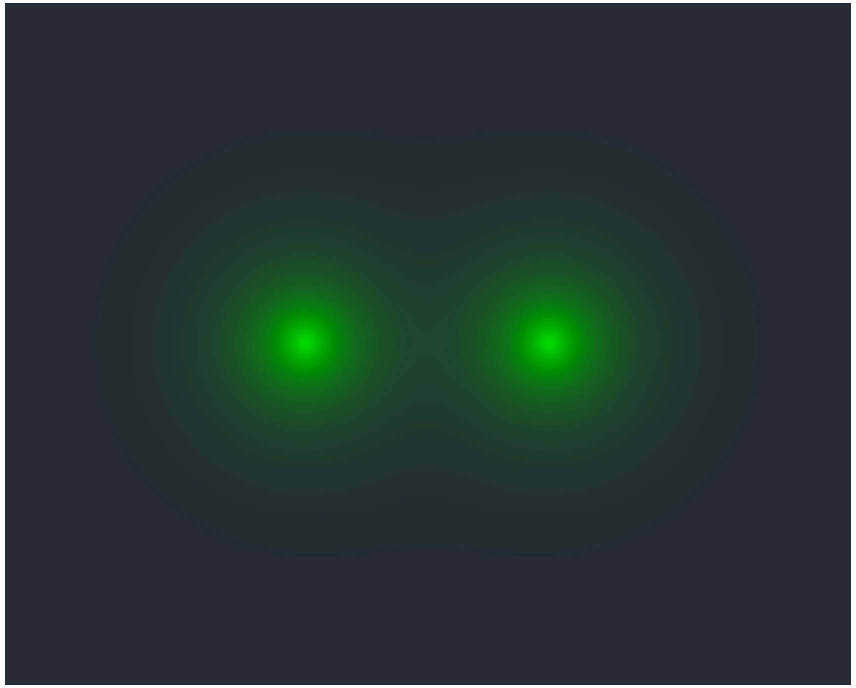
- Human enzymatic processes occur at room temperature
  - they come to a halt at freezing temperatures
- Many fish such as cod thrive in ice cold water
  - In what way differ their enzymes from ours?



Rare gasses

- Rare gases are inert — they are also called inert gases or noble gases
  - rare-gas atoms do not bind to other atoms



- Helium is the second most abundant element in the universe
  - one nucleus and two electrons
- The helium dimer He_2 exists but not as a chemical molecule
  - no accumulation of electrons between the nuclei

Stop press — new bond!

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- We discovered in 2012 that atoms bind in new ways in strong magnetic fields
  - stable rare-gas molecules
  - magnetic fields much stronger than what exists on Earth
  - ultra-strong fields occur on white dwarf stars and on neutron stars

Perpendicular paramagnetic bond

From Wikipedia, the free encyclopedia

A **perpendicular paramagnetic bond** is a type of chemical bond (in contrast to covalent or ionic bonds) that does not exist under normal, atmospheric conditions.[1] Such a phenomenon was first hypothesized through simulation to exist in the atmospheres of white dwarf stars[2] whose magnetic fields, on the order of 10^5 teslas,[1] allow such interactions to exist. Normally, at such intense temperatures as those near a white dwarf, more common molecular bonds cannot form and existing ones decompose.[2]

References [edit]

1. ^ a b Lange, K. K.; Tellgren, E. I.; Hoffmann, M. R.; Helgaker, T. (19 July 2012). "A Paramagnetic Bonding Mechanism for Diatomics in Strong Magnetic Fields". *Science*. **337** (6092): 327–331. Bibcode:2012Sci...337..327L. doi:10.1126/science.1219703. PMID 22822146.
2. ^ a b Yirka, Bob (July 20, 2012). "Chemists discover new type of molecular bond near white dwarf stars". *phys.org*. Retrieved 2018-12-24.

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Rewriting the rules of the universe: Mysterious new atomic bond found in white dwarf stars could change computing forever

- Third kind of bond after ionic and covalent
- Found only in white dwarf stars - with magnetic stronger than any on Earth
- Find rewrites rules of universe
- Could lead to new discoveries in quantum phys
- Techniques used to analyse bonds could lead t

By ROB WAUGH

PUBLISHED: 11:07 GMT, 24 July 2012 | UPDATED: 11:24 GMT, 24 July 2012

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A new kind of bond between atoms found only in the crushingl dwarf stars could unlock new secrets of quantum physics.

The find - a 'third kind' of bond between atoms, unknown on E ultra-powerful new computers.

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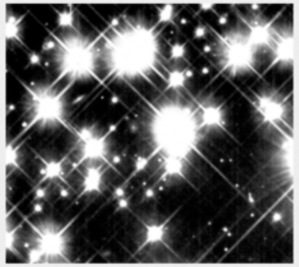

White Dwarf Stars This image from the Hubble Space Telescope shows a close-up of ancient white dwarf stars in the Milky Way.

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BY DAN NOSOWITZ POSTED 19.07.2013 | 1 COMMENT

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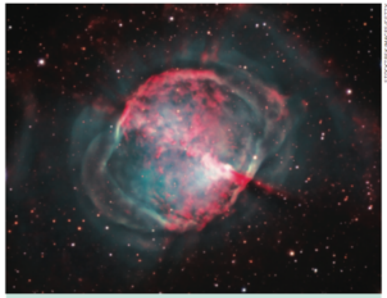
BY DAN NOSOWITZ POSTED 13.07.2013 | 3 COMMENTS

Science



A bond that can only form in space

THERE'S a new bond in town, and this secret agent works best in extreme situations. The chemical bond occurs in the presence of strong magnetic fields, such as those found around white dwarfs, the remnant cores of dead, low-mass stars. Earth's field is too puny for it to happen here.

Because the electrons in atomic bonds follow the Pauli principle – two of them cannot occupy the same quantum state – they pair up in couples of opposing spin. If the spins of both become aligned, one is forced into a so-called anti-bonding orbital. "The atoms are no longer bound together and the molecule breaks apart," says Kai Lange at the University of Oslo in Norway.

But when Lange and colleagues simulated bonding in hydrogen and helium atoms in the magnetic field of a white dwarf – 10 billion times greater than Earth's – the atoms were drawn into strongly bonded pairs in both cases. Because the electrons occupied the anti-bonding orbitals yet bonded together, it's a new type of chemical bond (*Science*, DOI: 10.1126/science.1219703). The space-only bond shows chemistry changing under extreme conditions.

28 July 2012 | NewScientist | 15

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NATURE | NEWS

Stars draw atoms closer together

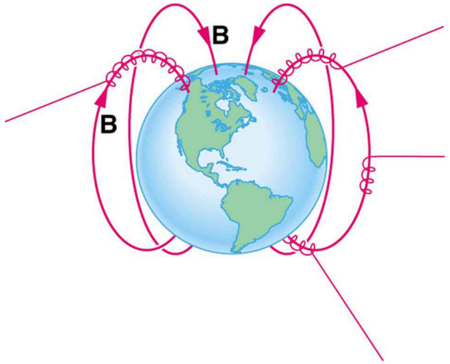
Previously unknown bonding mechanism predicted in magnetic fields of white dwarfs.

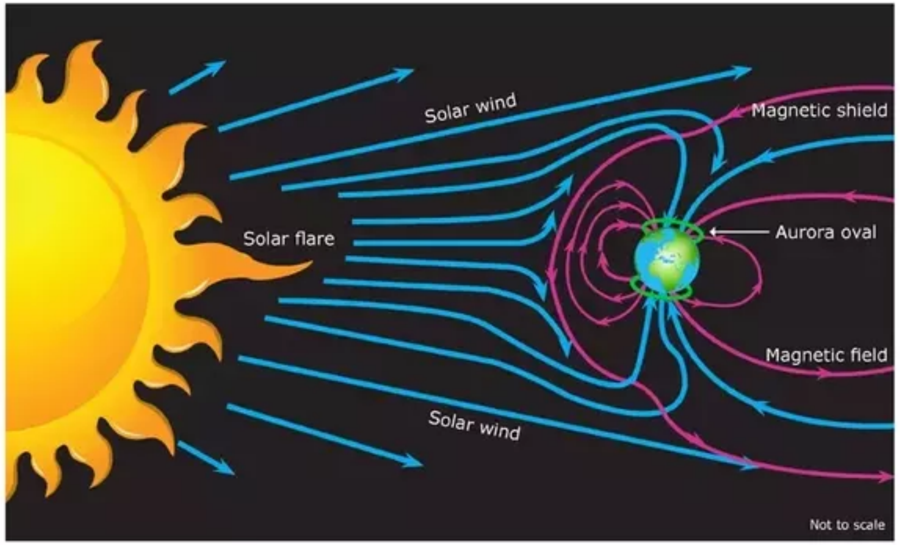
Zeeya Merali

19 July 2012

Electrons in a magnetic field

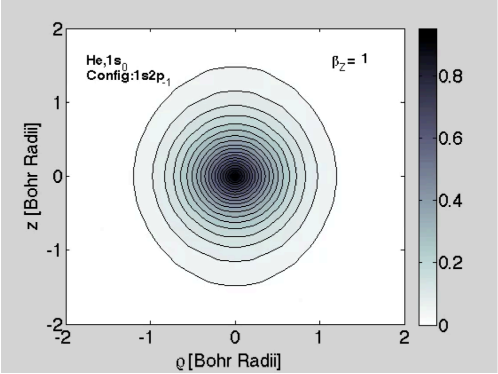
- A magnetic field influences the motion of electrons
  - the magnetic field of the Earth protects us against radiation
  - how are electrons inside a molecule affected by a magnetic field?

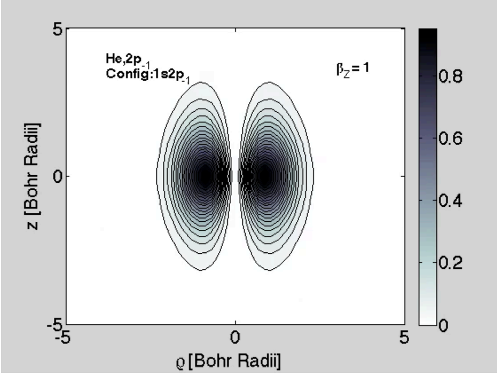


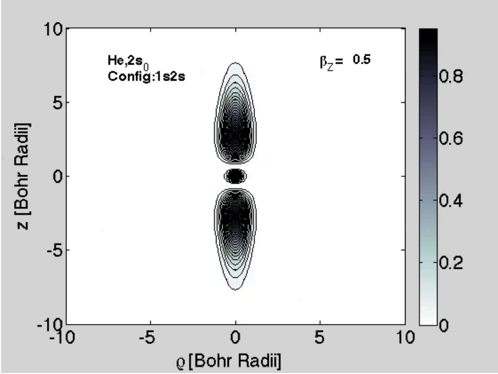


(Extra)terrestrial chemistry

- Earth: 0 – 100 T — familiar chemistry
  - electric forces dominate
- White dwarfs: 0 – 100 kT — exotic chemistry
  - magnetic and electric forces compete
- Neutron stars: 1 – 100 GT — alien chemistry
  - magnetic forces dominate

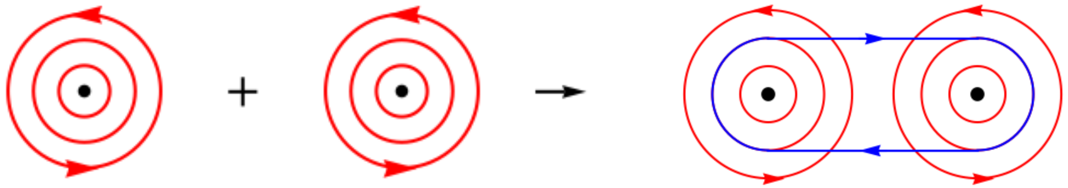


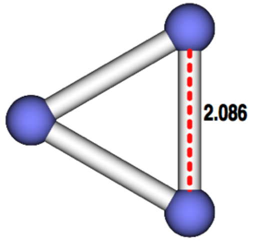


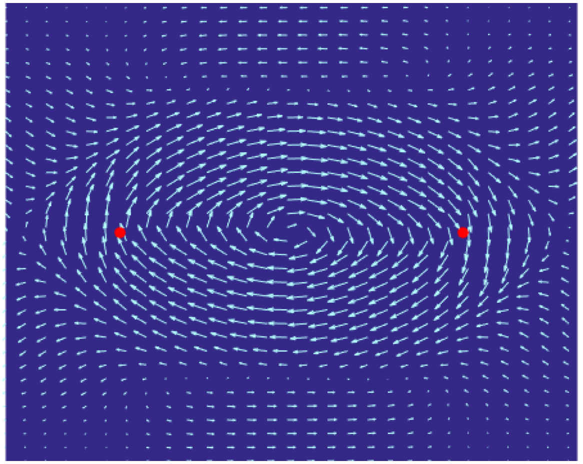


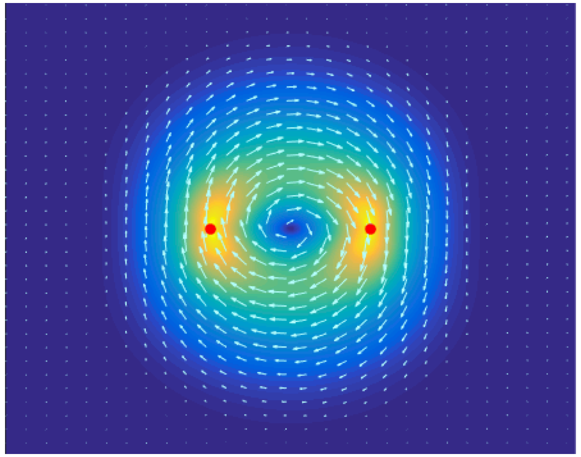
Magnetic bonding

- A magnetic field sets up anti-clockwise currents in each helium atom
  - these currents increase the energy of the atoms
- When the atoms come close together, counter currents are induced in the molecule
  - these currents reduce the energy, effectively binding the atoms into a stable molecule









Magnetically induced currents in helium dimer

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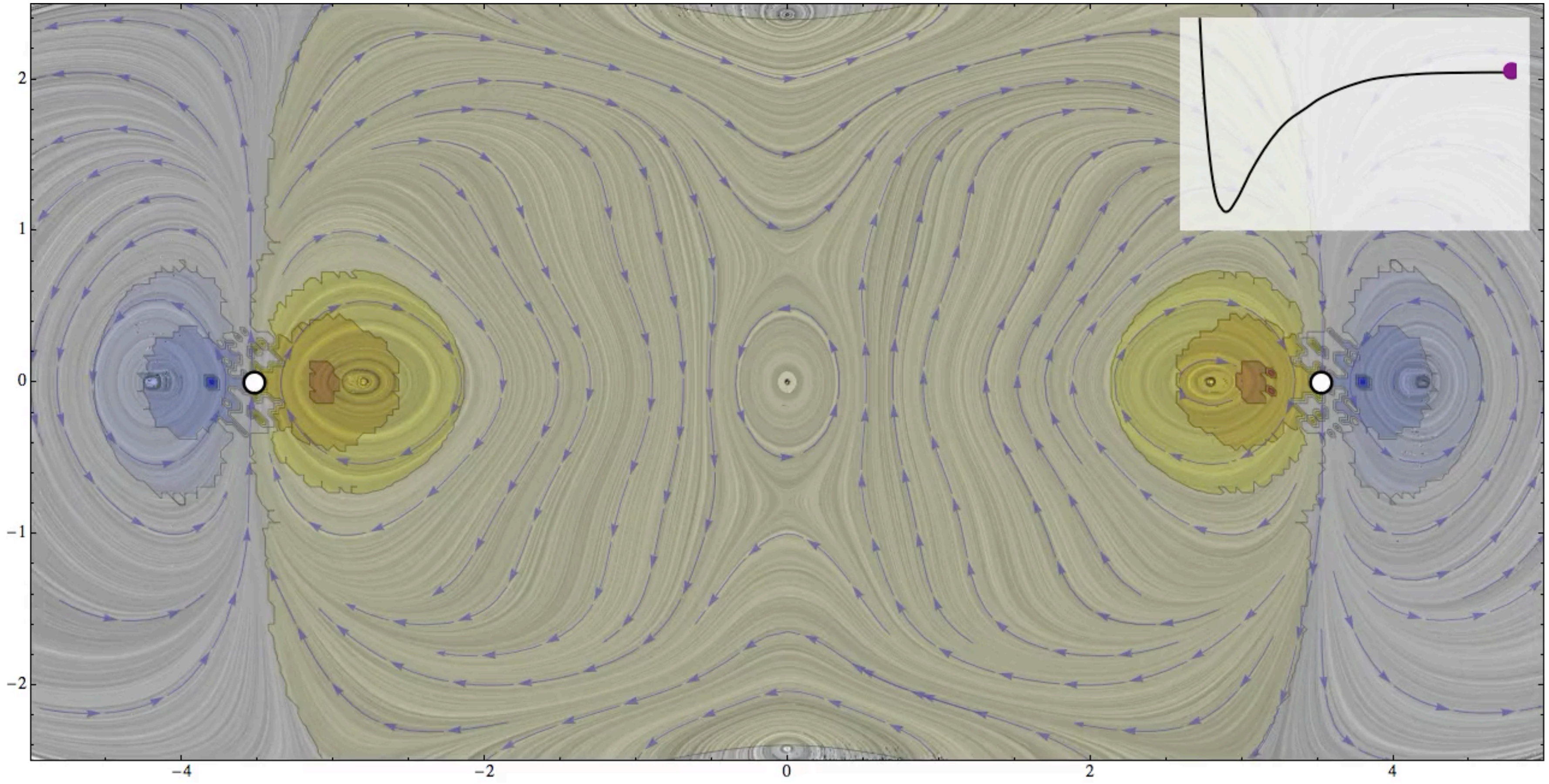
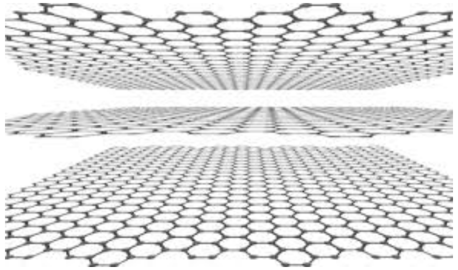
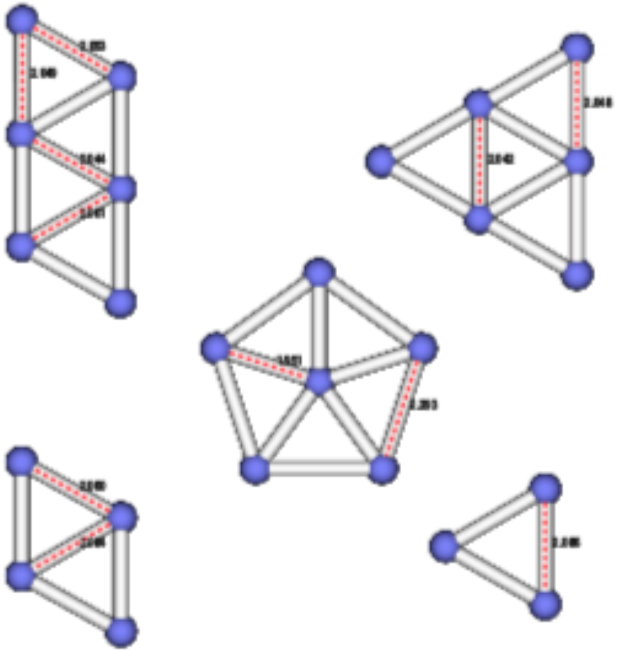
- The helium molecule arises as a compromise between two effects
  - magnetic forces pull atoms together — electric forces push them apart



Helium flakes

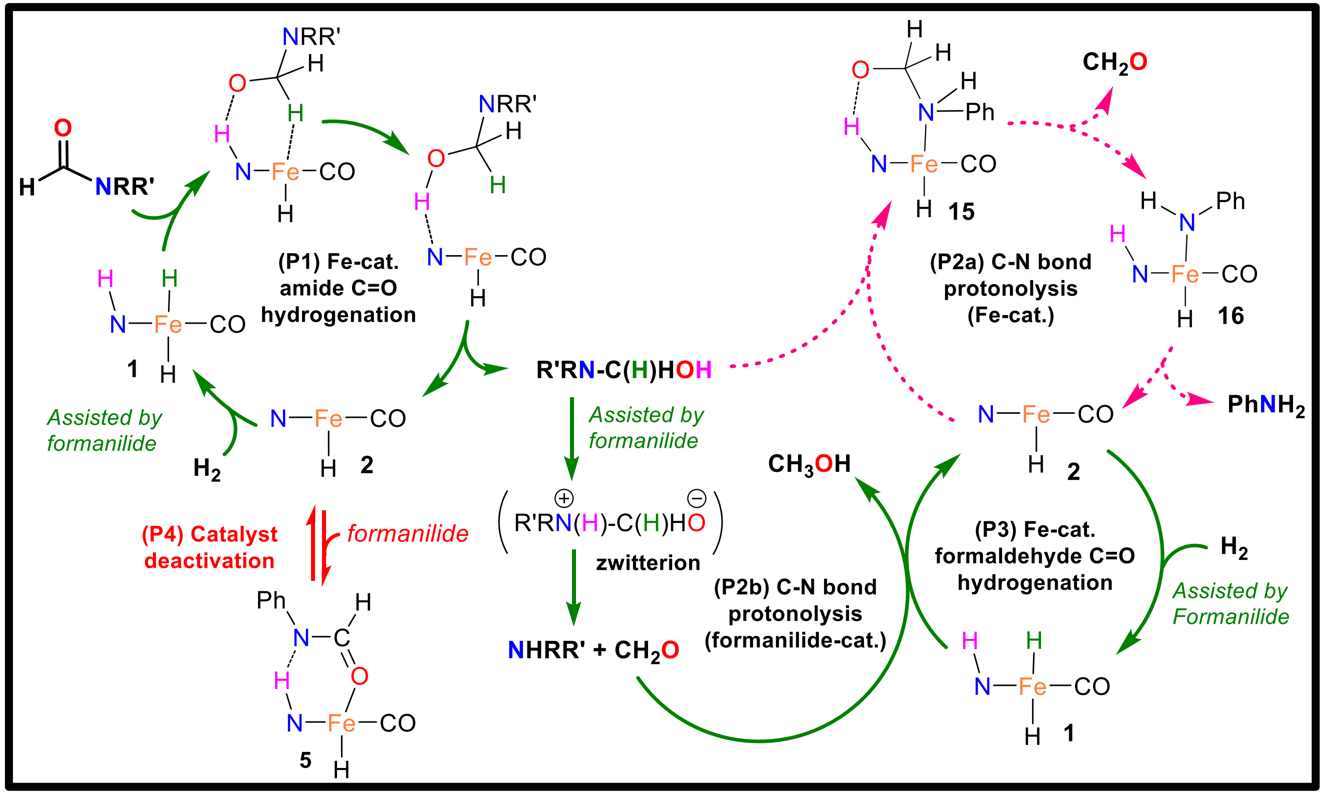
- Magnetic binding generates flakes of helium atoms
  - structure reminiscent of 2D hexagonal crystals generated under extreme pressure





Chemical transformations

- Methanol valuable chemical — expensive to produce
- Net reaction: $CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$
- In practice, production is much more complicated — here from amide by means of catalysts
- The following catalytic mechanism using an iron catalyst has been mapped out



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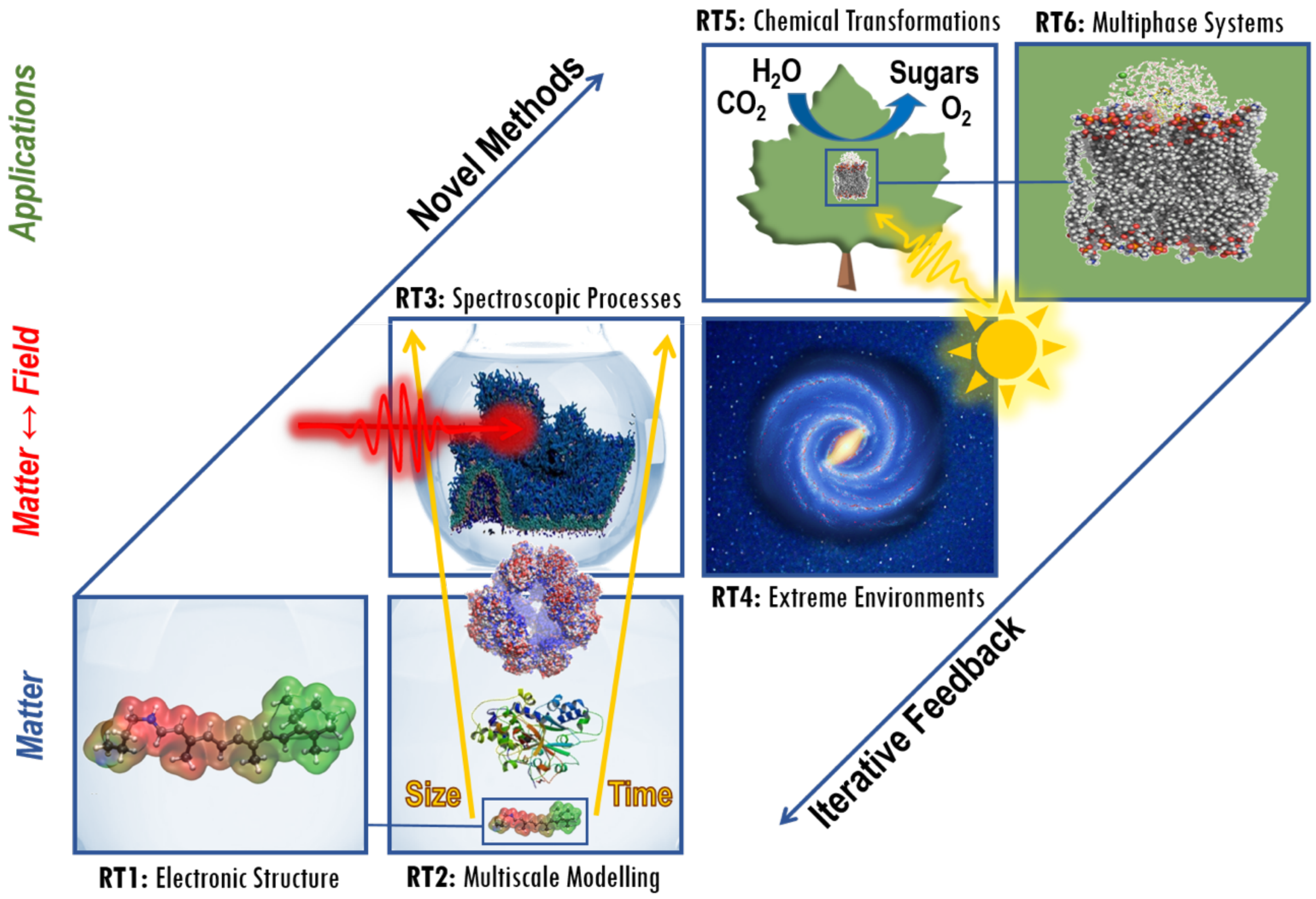
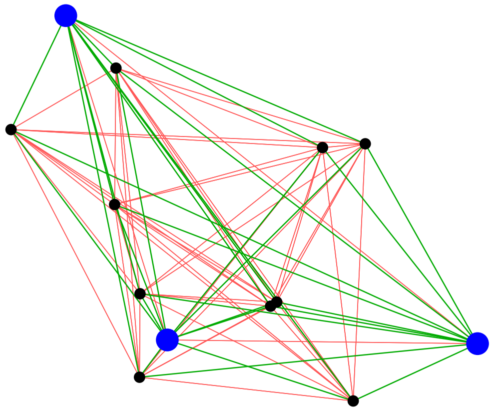
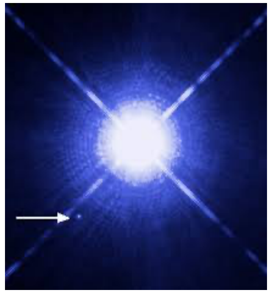


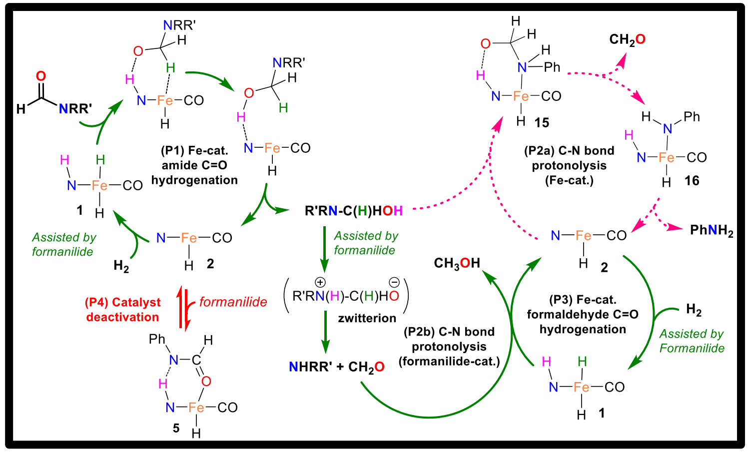
Quantum Chemistry — a Matter of Life an Death

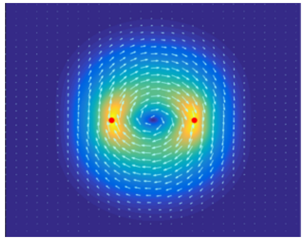
Hylleraas

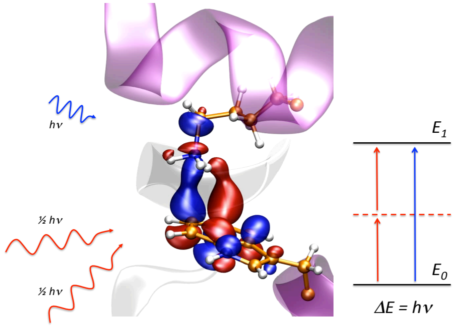
- Quantum chemistry — a versatile, generic tool
  - gives insight into processes in living and dead matter
  - From the delicate human eye to the fierce white-dwarf atmospheres
- Chemistry — the central science
  - physics — chemistry — biology











Our vision

The Hylleraas Centre will develop and apply computational methods to understand, interpret, and predict new chemistry, physics, and biology of molecules in complex and extreme environments