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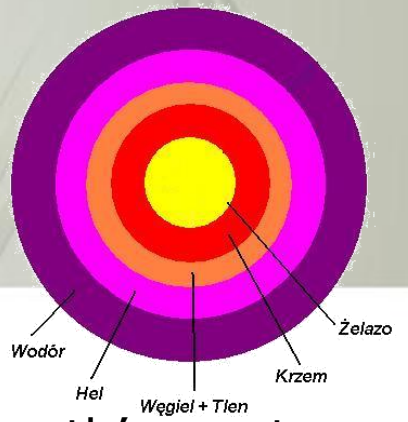
Chemistry of Coal

Physical chemistry of carbonaceous materials

Faculty of Energy and Fuels

Krakow, 2012

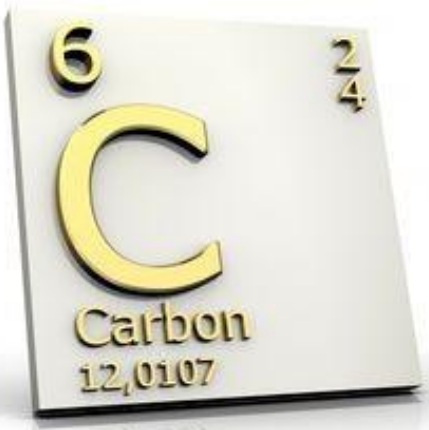
Carbon

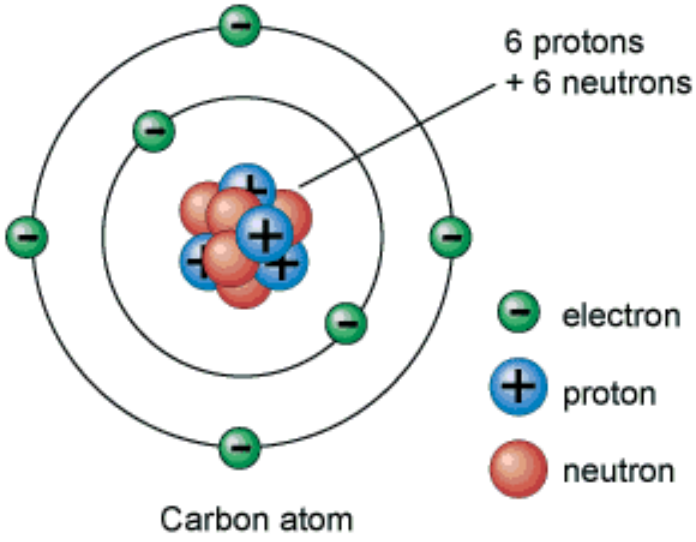


- 4-th place in diffusion in space
- 14-th element in the view of currency in the earth's crust
- content in biotic world (living world) is 100 time bigger than in abiotic (non-living) but non in global values
- a) atom weight – $1.992 * 10^{-23}$ g/atom
  b) atomic mass – 12 a.m.u.
- molar mass – 12.01 (98.9% isotope ^{12}C and 1.1% isotope ^{13}C in the earth crust, ^{14}C 1 pbb)
- carbon is unsoluble in water, acids and bases but is soluble in metals and alloys (e.g. in iron – making a solid state solution called steel)
- 1/12 of isotope ^{12}C mass is set up as an atomic mass unit (a.m.u.) standard

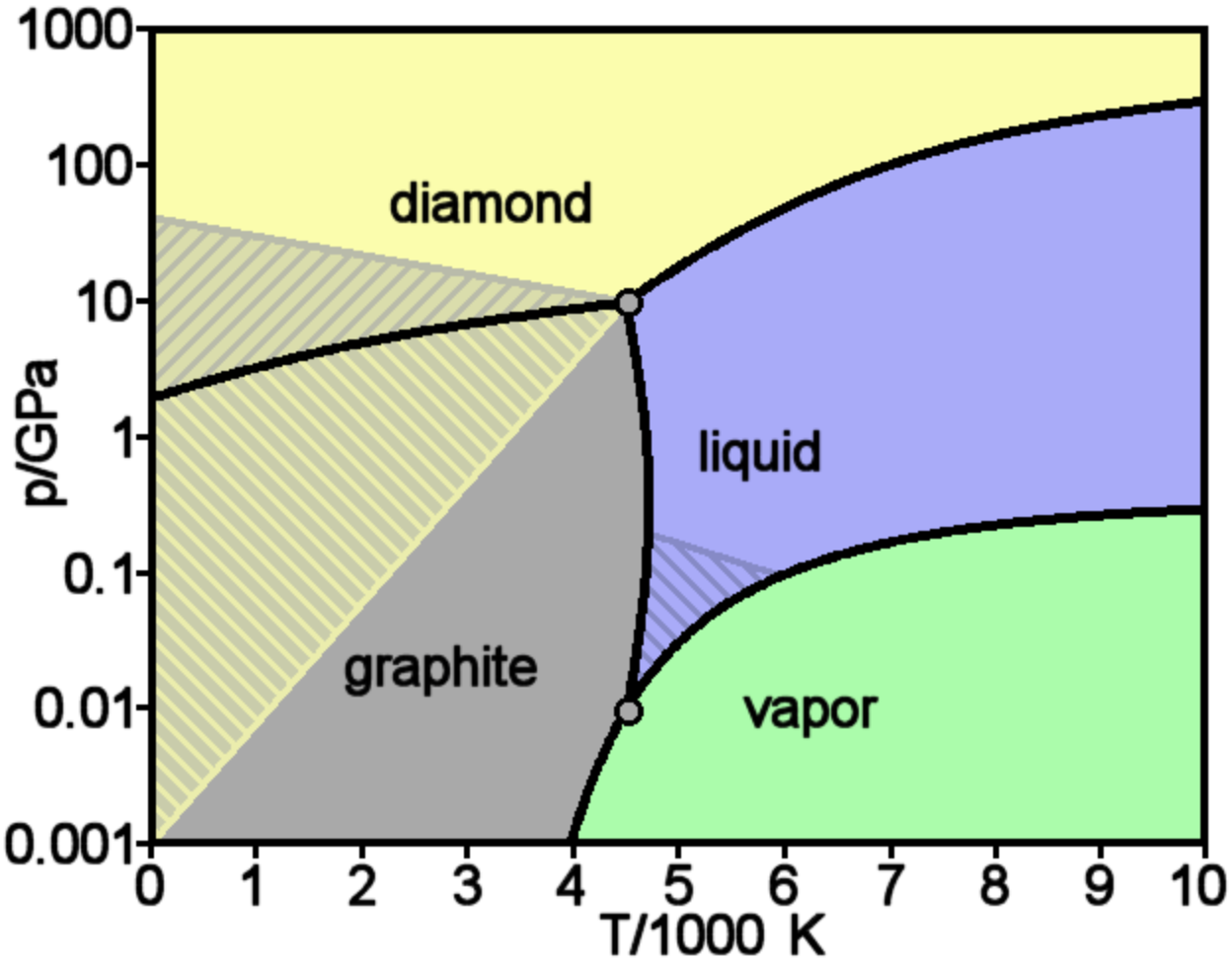
Carbon

- specific properties of carbon:
  - **C-C bound H= 348 kJ/mol**
  - Si-Si bound H= 226 kJ/mol
  - N-N bound H= 160 kJ/mol
  - O-O bound H= 147 kJ/mol

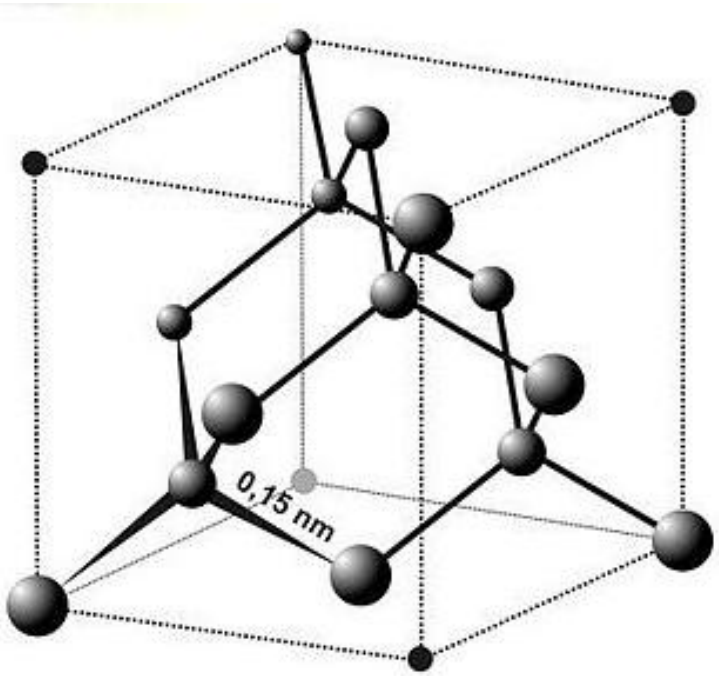


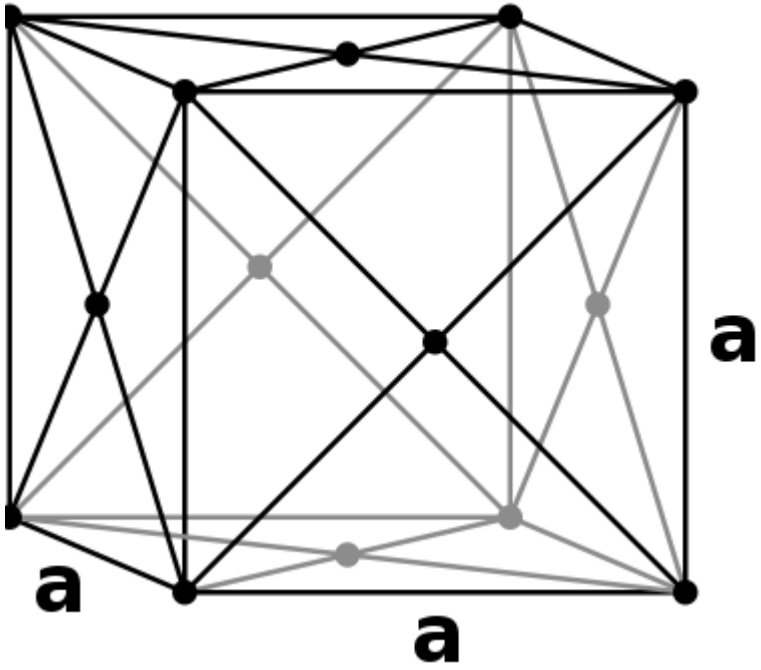


Carbon - allotropes

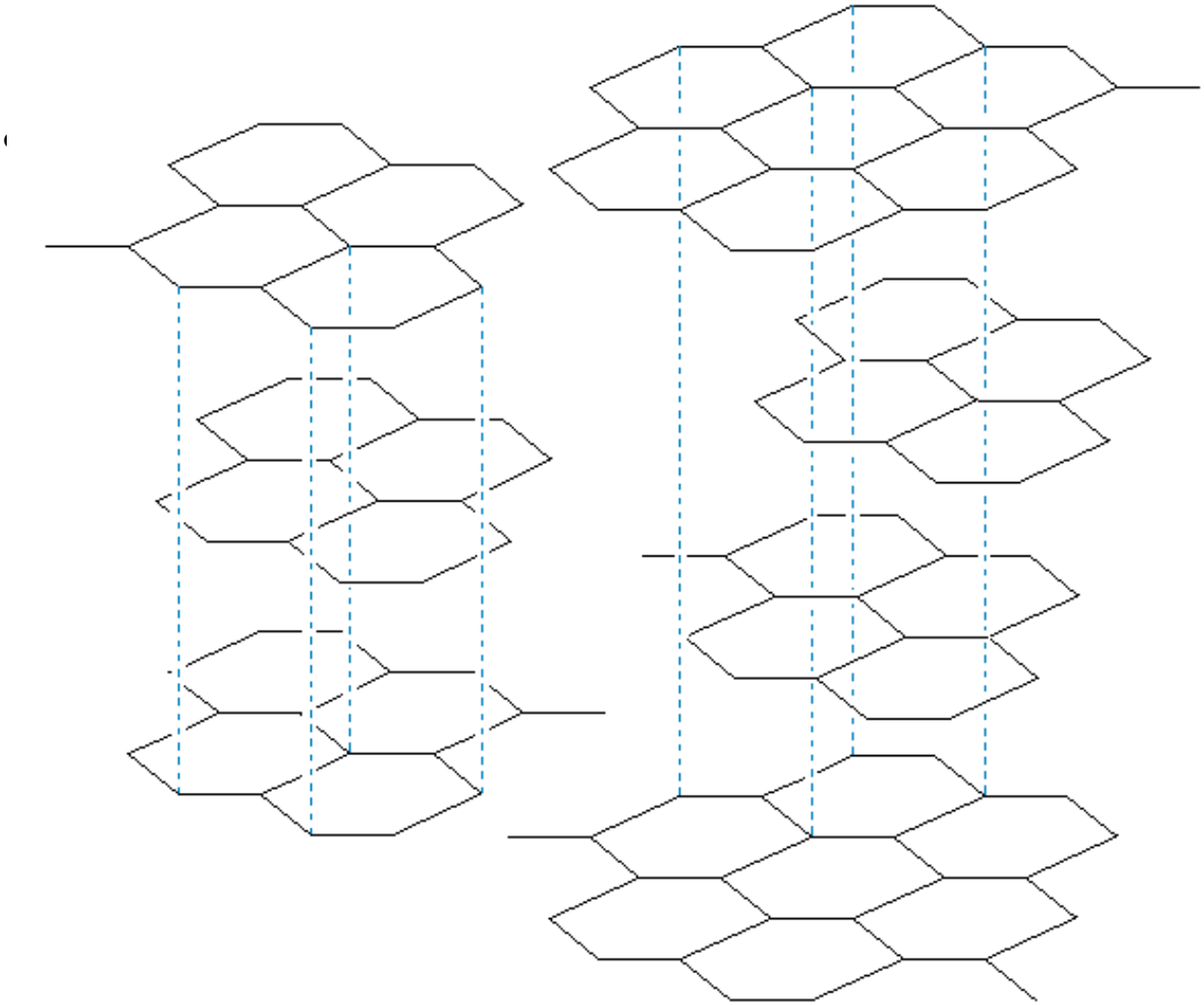


Carbon – allotropes - diamond





Carbon – allotropes - graphite



Carbon – allotropes - graphite

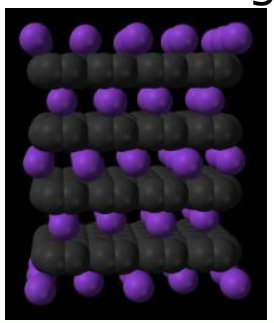
Modified graphite

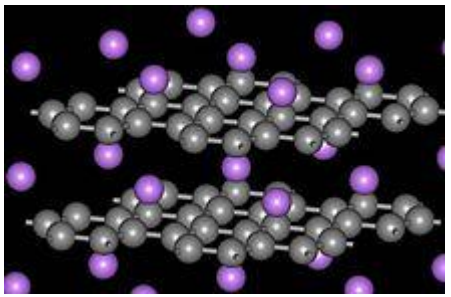
- expanded

  after immersing natural flake graphite in a bath of chromic acid, then concentrated sulfuric acid, which forces the crystal lattice planes apart

  improves fireproofing – foundry, fire-stoping doors, fire-proof paints (lacquers), fire-proof gaskets, fuel cells
- intercalated

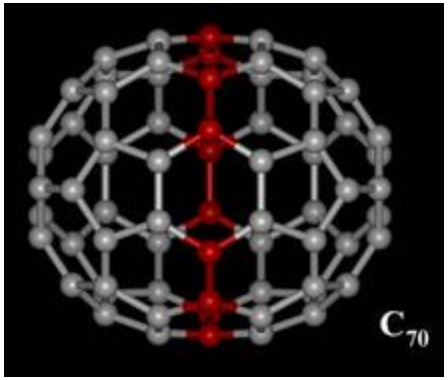
  introducing of some metals or small molecules (Ca, Sr, Li, K, Rb, Cs, carbon fluorides, graphite bisulfate and graphite perchlorate and others)

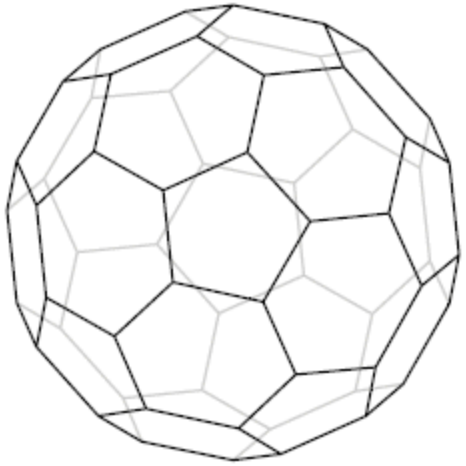




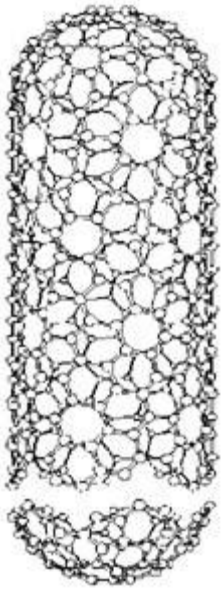
Carbon - allotropes

- Fullerens (from the name Buckminster Fuller – BuckyBalls)
  atoms are arranged in a space, spherical-like shape
  depend on number of carbon atoms in structure
  atoms distance 0.144 nm (C60 fullerene)
  Density: 1.72 g/cm^3
  bulk modulus: 14 Gpa
  thermal and electrical rather insulating



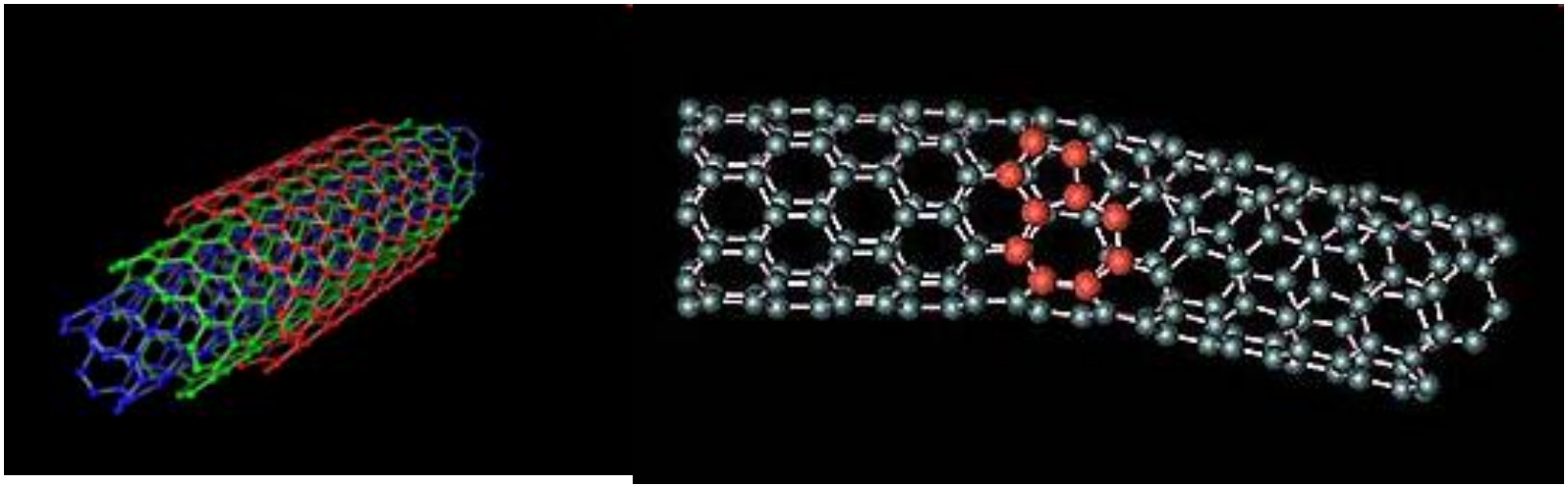


Carbon – allotropes - nanotubes

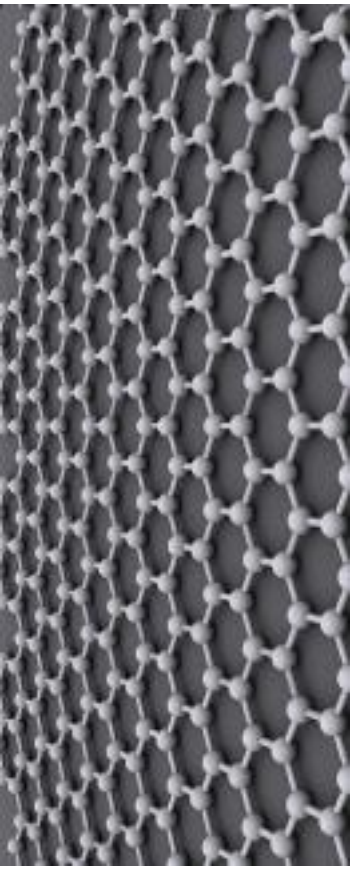


- Nanotubes – single walled
  (some sais subcathegory of fullerenes)
  atoms are arranged in a space shape depend on number of carbon atoms in structure
  atoms distance 0.142 nm, opposite atoms 0.283 nm
  Density:

Zigzag	1.33 g/cm^3
Armchair	1.34 g/cm^3
Chiral	1.40 g/cm^3



Carbon – allotropes - graphene



- Graphene – one-atom planar sheets of sp^2-bonded carbon atoms lattice, looks like honeycomb

  atoms distance 0.142 nm,

  tensile strength: 1 Tpa (more strength material known)

  heat transfer: 5000 $Wm^{-1}K^{-1}$

  electricaly: semi-metal – semi-conductors

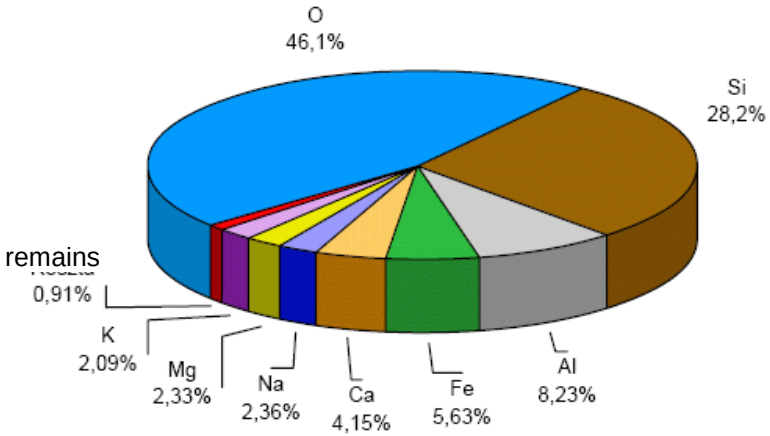
  opticaly: one-atom layer absorbs 2,3% of light

  Use: room temperature alcohol distilation, single molecule gas detection, FET transistors (integrated circuits), optical modulators, transparent conducting electrodes, solar cells, supercapacitors, graphene oxide paper (insulator, conductor and semiconductor)

Carbon – occurence in nature

Carbon content [bilion tonns] from A.E.Fersman	
living organisms	700
earth	400
peat	1 200
lignites	2 100
hard coals	3 200
anthracites	600
sedimentary rocks	4 576 000
oceans, seas and rivers	184 000
atmosphere	2 200

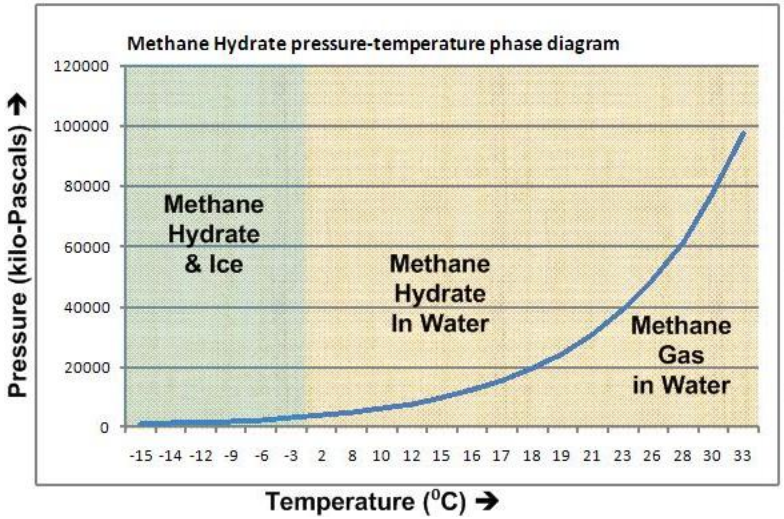
living organisms		earth crust	
element	%	element	%
oxygen	65	oxygen	49.5
carbon	18	silicon	25.5
hydrogen	10	aluminium	7.5
nitrogen	3	iron	5
calcium	2	calcium	3.4
phosphor	1	sodium	2.6
K, S, Cl, Na, Mg, Fe	0.9	hydrogen	0.8
		Ti, Cl, P	0.6

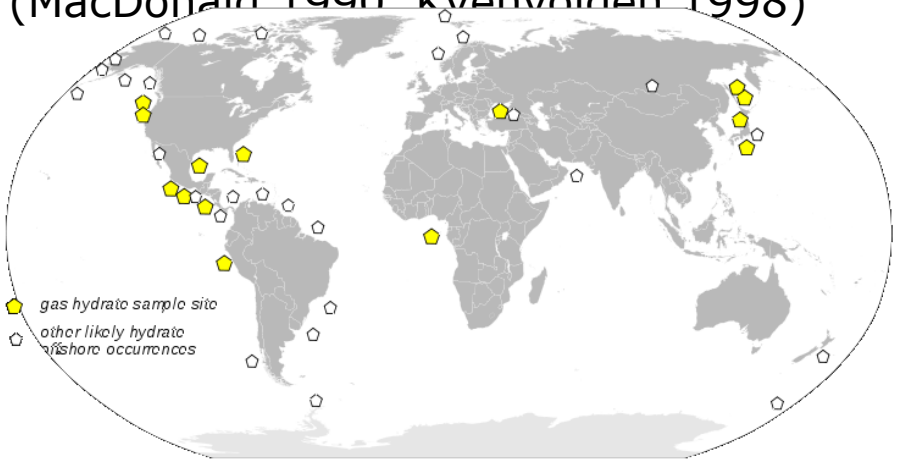


Carbon – natural occurence methane clathrate

Methane clathrate, methane hydrate, methane ice

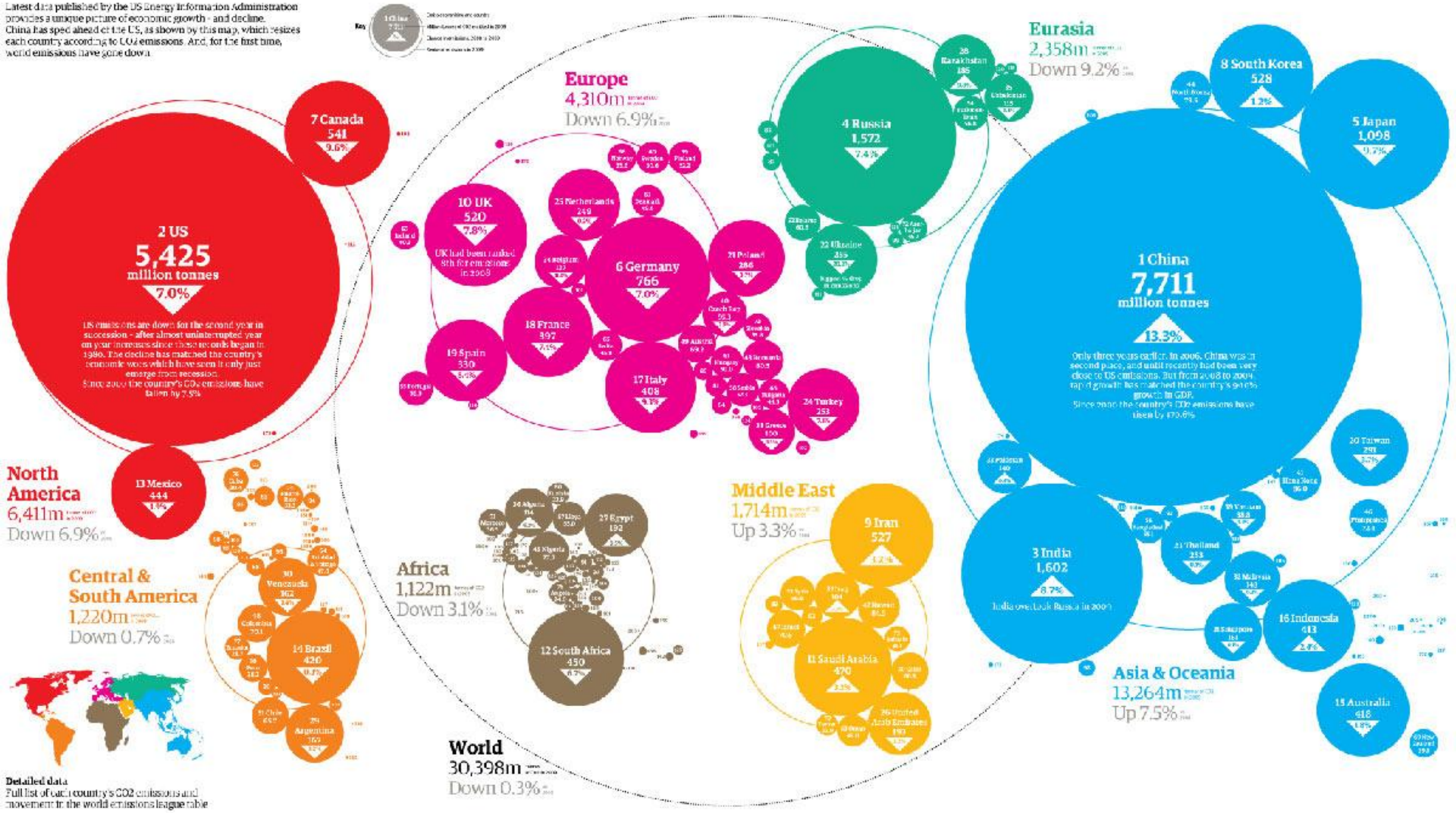
- gas hydrate – a solid clathrate compound in which a methane is trapped within a crystal structure of water, forming a solid similar to ice
- 1 mole of methane for 5.75 moles of water
- natural deposites – shallow lithosphere < 2000 m depth
- appears in less than 0°C and 300 m of water layer
- 10 000 to 11 000 Gt (MacDonald 1990, Kvenvolden 1998)





An atlas of pollution: the world in carbon dioxide emissions

Latest data published by the US Energy Information Administration provides a unique picture of economic growth – and decline. China has sped ahead of the US, as shown by this map, which resizes each country according to CO2 emissions. And, for the first time, world emissions have gone down.



Detailed data
Full list of each country's CO2 emissions and movement in the world emissions league table

Carbon cycle

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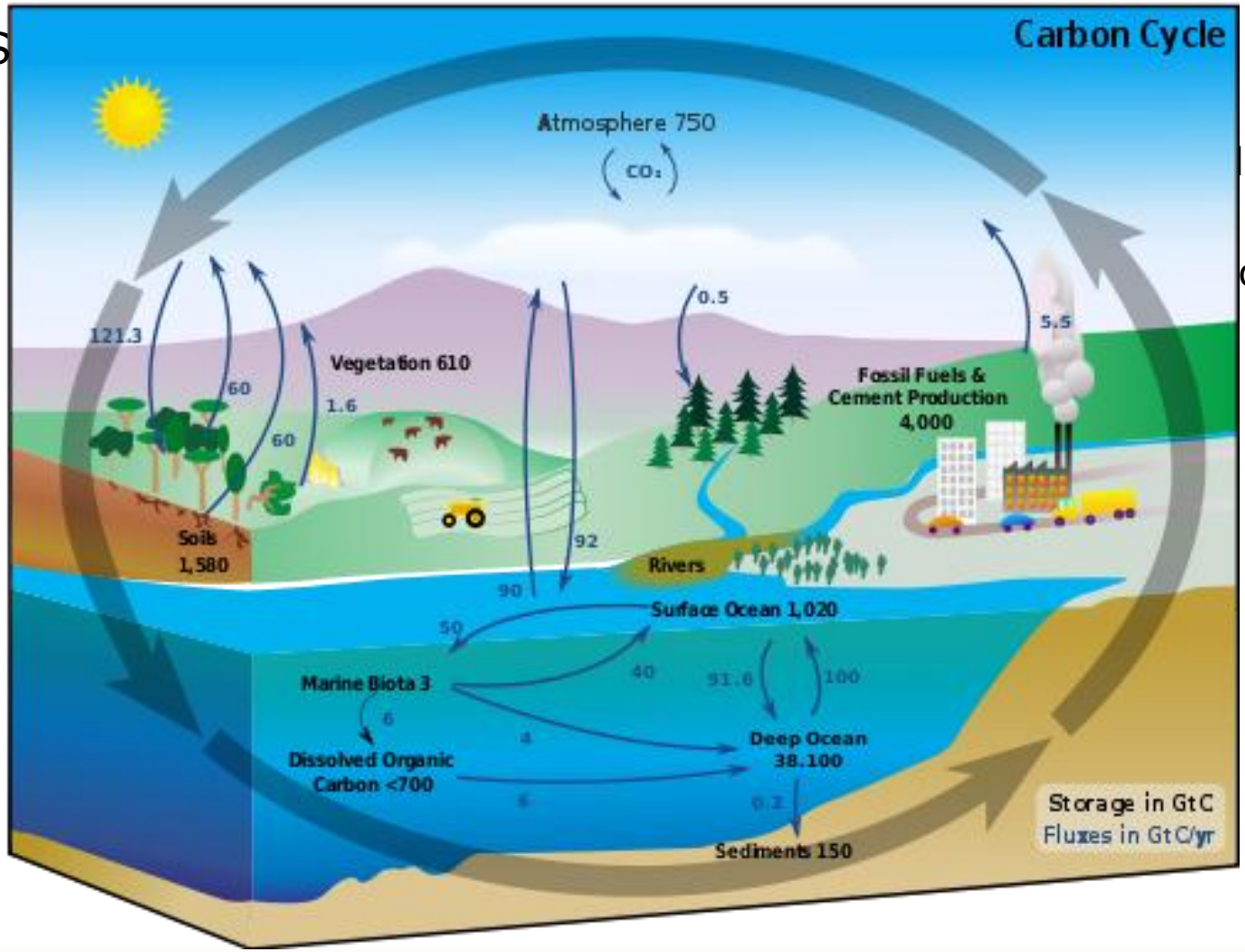
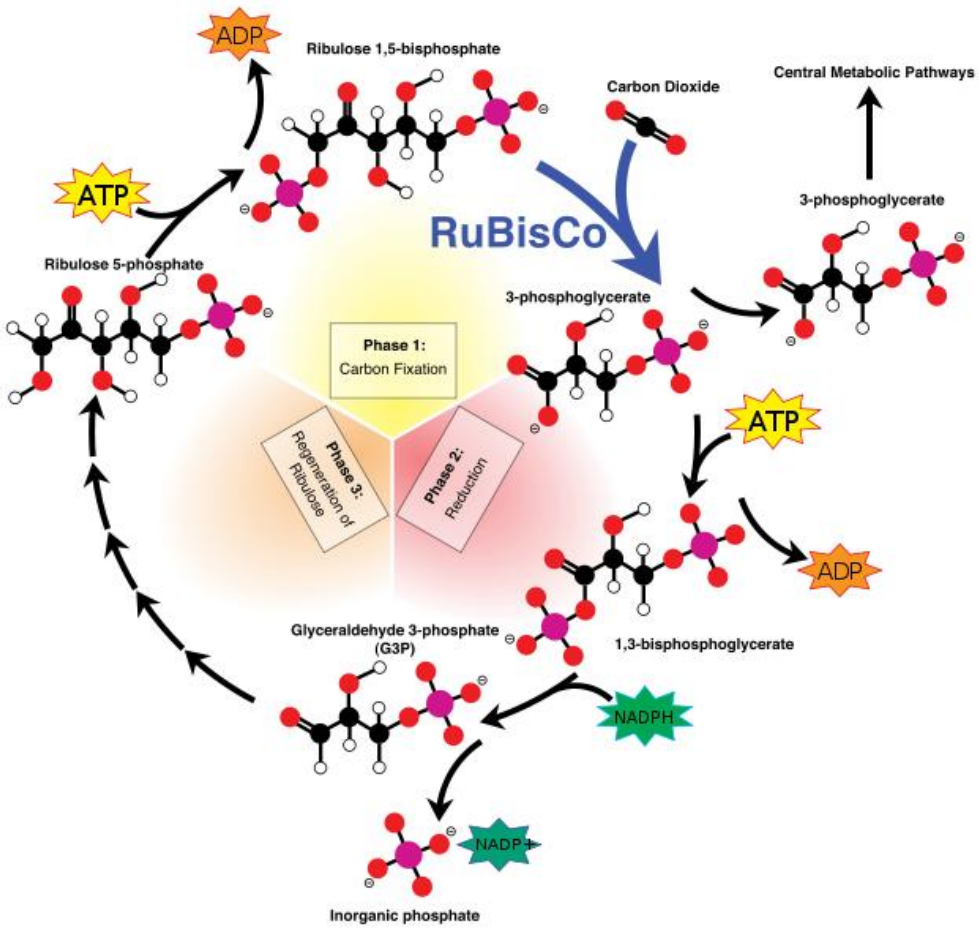


Calvin Cycle

Calvin cycle, C3 cycle or Calvin–Benson-Bassham (CBB)

- series of biochemical redox reactions that take place in the in photosynthetic organisms
- reductive pentose phosphate cycle
- two stage:
  - light-dependent – energy storage ATP and NADPH
  - light-independent – energy use for water and organic organic compound production from CO2



Krebs Cycle

citric acid cycle, tricarboxylic acid cycle (TCA cycle),

Krebs cycle,

Szent-Györgyi–Krebs cycle

- series of chemical reactions used by all aerobic organisms to generate energy through the oxidization of acetate derived from carbohydrates, fats and proteins into carbon dioxide and water
- provides precursors for the biosynthesis of compounds used in numerous bio-reaction