



**AKADEMIA GÓRNICZO-HUTNICZA  
IM. STANISŁAWA STASZICA W KRAKOWIE**

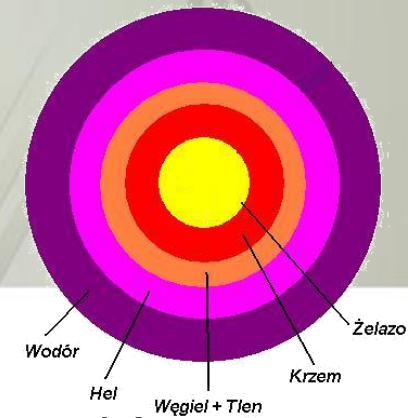
# **Chemistry of Coal**

**Physical chemistry of carbonaceous materials**

**Faculty of Energy and Fuels**

**Krakow, 2012**

# Carbon

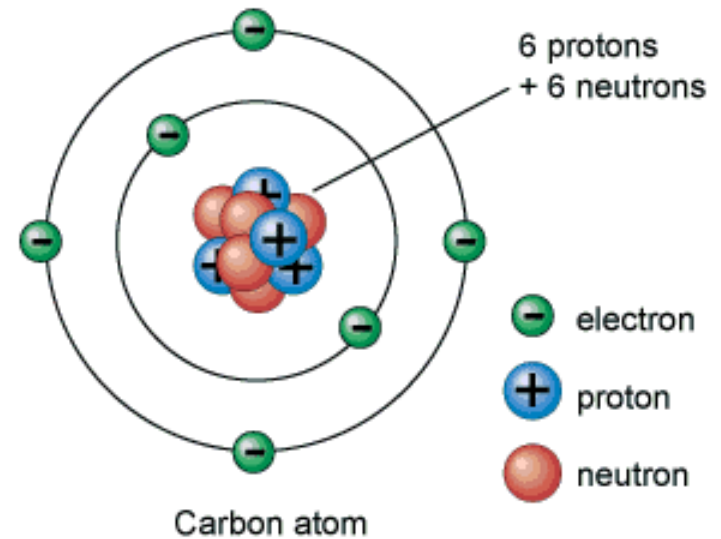


- 4-th place in diffusion in space
- 14-th element in the view of currency in the earth's crust
- content in biotic world (living world) is 100 time bigger than in abiotic (non-living) but non in global values
- a) atom weight –  $1.992 \cdot 10^{-23}$  g/atom  
b) atomic mass – 12 a.m.u.
- molar mass – 12.01 (98.9% isotope  $^{12}\text{C}$  and 1.1% isotope  $^{13}\text{C}$  in the earth crust,  $^{14}\text{C}$  1 pbp)
- 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  $^{12}\text{C}$  mass is set up as an atomic mass unit (a.m.u.) standard

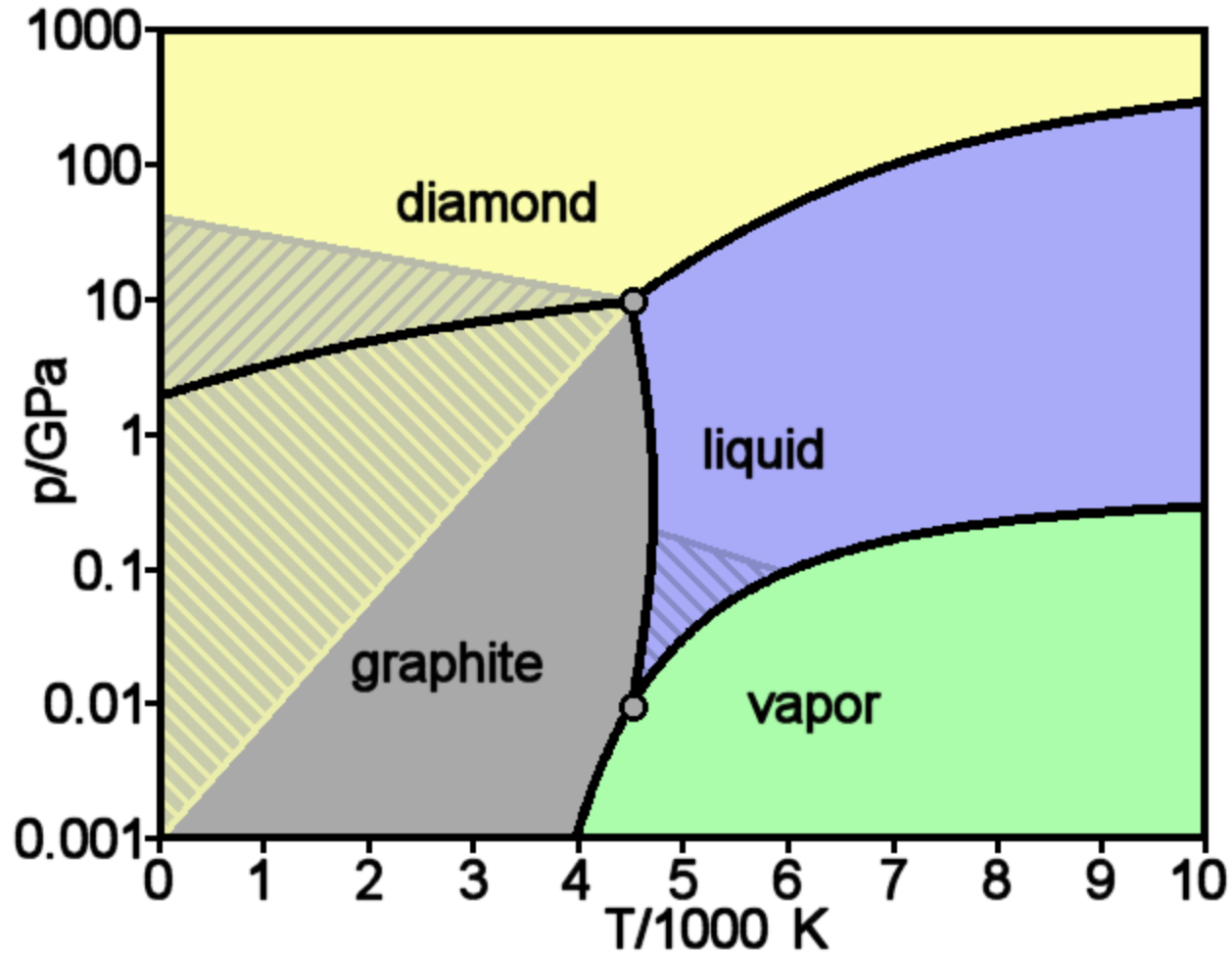


# Carbon

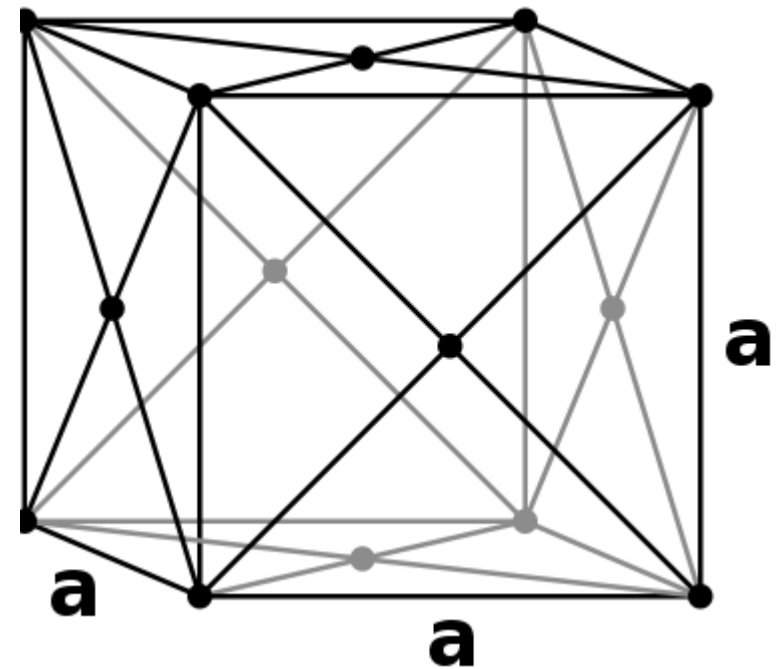
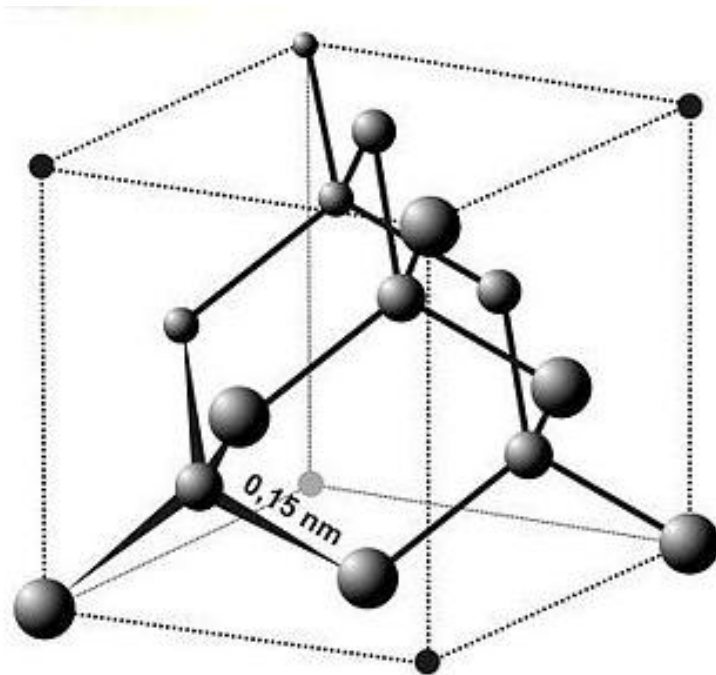
- specific properties of carbon:
  - **C-C bond H= 348 kJ/mol**
  - Si-Si bond H= 226 kJ/mol
  - N-N bond H= 160 kJ/mol
  - O-O bond H= 147 kJ/mol



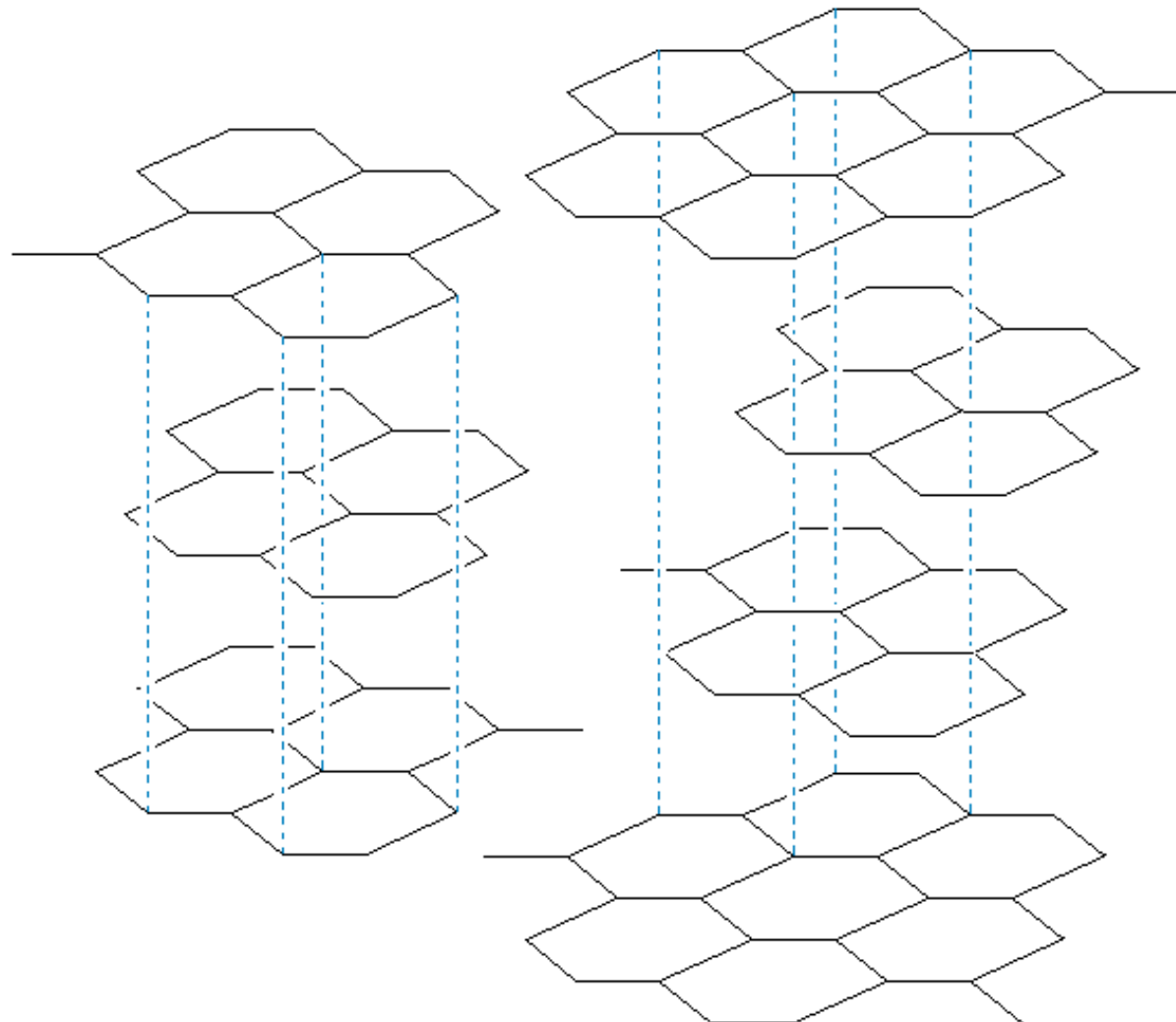
# Carbon - allotropes



# Carbon – allotropes - diamond



# Carbon – allotropes - graphite



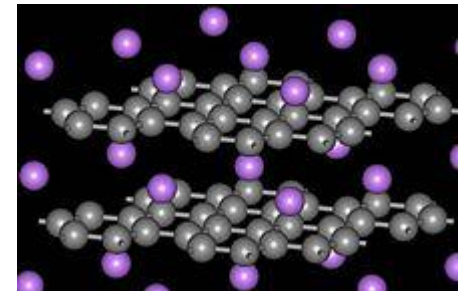
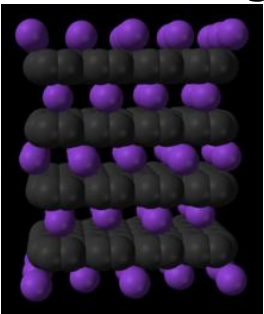
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# Carbon – allotropes - graphite

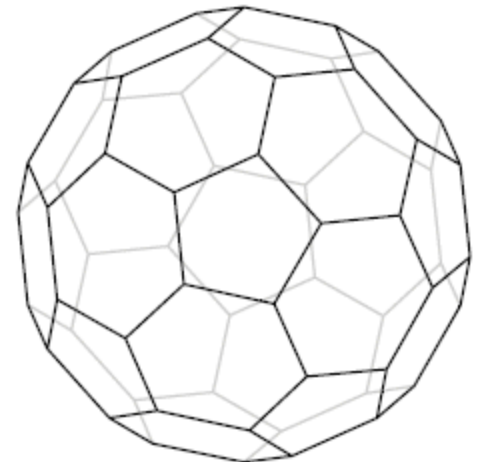
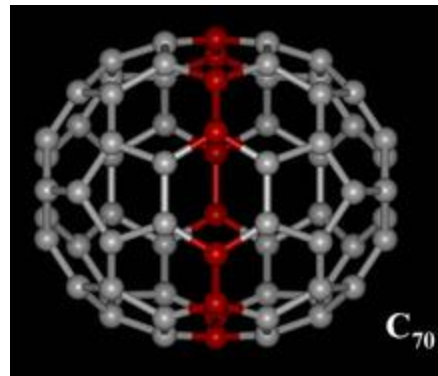
## Modified graphite

- 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-stopping 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<sup>3</sup>  
bulk modulus: 14 Gpa  
thermal and electrical rather insulating





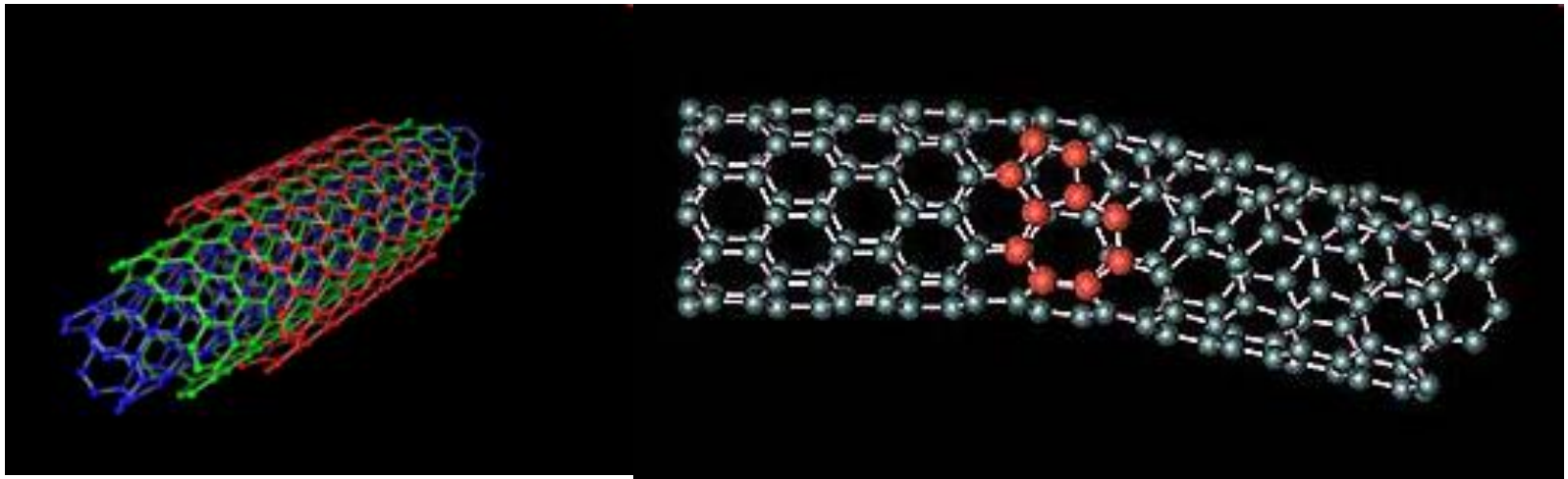
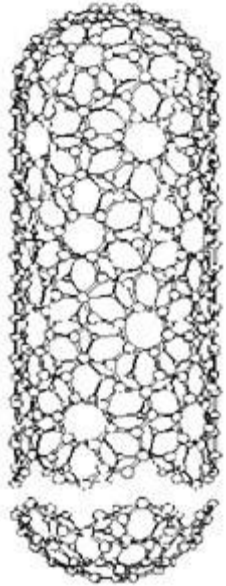
# Carbon – allotropes - nanotubes

- Nanotubes – single walled  
(some says subcategory 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

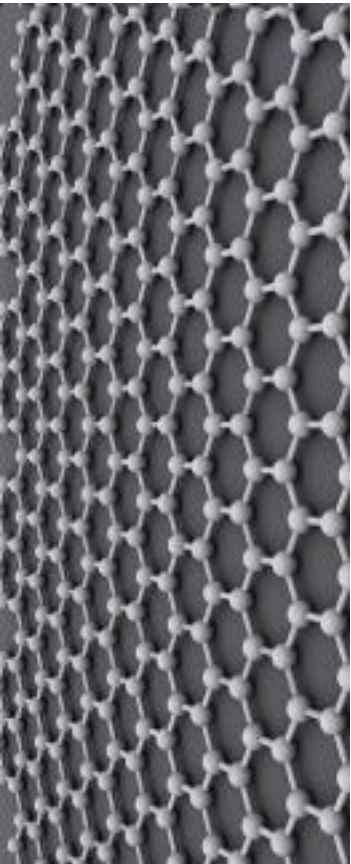
Density:

Zigzag	1.33 g/cm <sup>3</sup>
Armchair	1.34 g/cm <sup>3</sup>
Chiral	1.40 g/cm <sup>3</sup>



## Carbon – allotropes - graphene

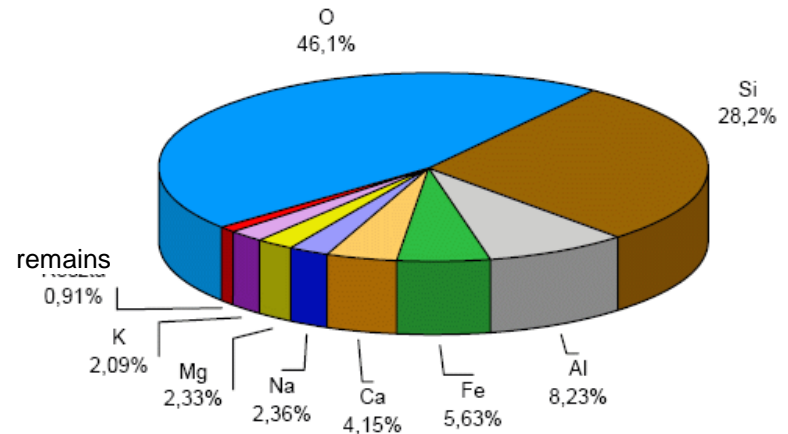
- Graphene – one-atom planar sheets of  $sp^2$ -bonded carbon atoms lattice, looks like honeycomb  
atoms distance 0.142 nm,  
tensile strength: 1 Tpa (more strength material known)  
heat transfer:  $5000 \text{ Wm}^{-1}\text{K}^{-1}$   
electrically: semi-metal – semi-conductors  
optically: one-atom layer absorbs 2,3% of light  
Use: room temperature alcohol distillation, single molecule gas detection, FET transistors (integrated circuits), optical modulators, transparent conducting electrodes, solar cells, supercapacitors, graphene oxide paper (insulator, conductor and semiconductor)



# Carbon – occurrence 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

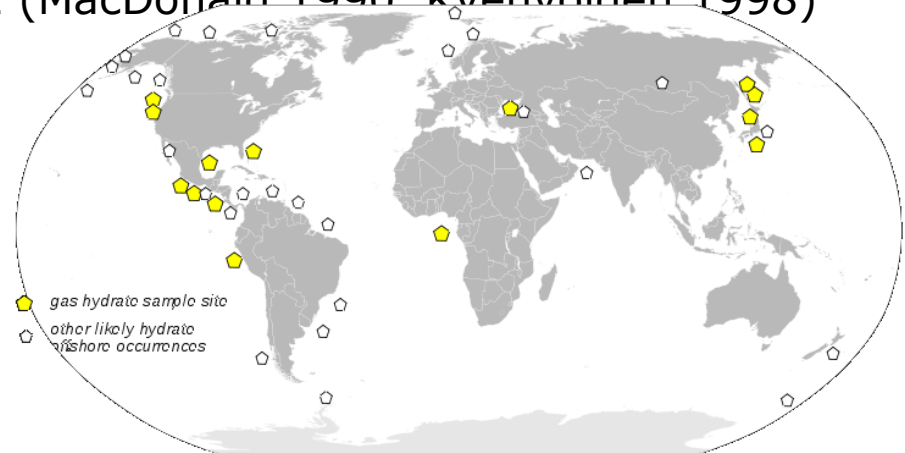
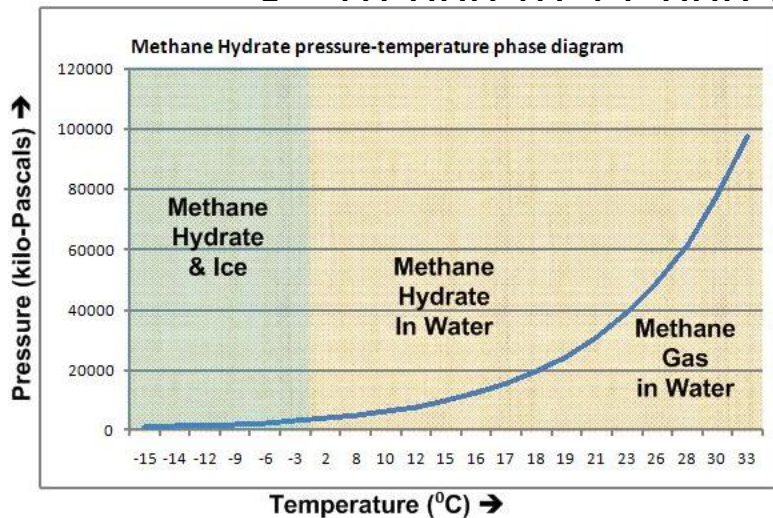
living organisms		earth crust	
element	%	element	%
oxygen	65	oxygen	49.5
carbon	18	silicon	25.5
hydrogen	10	aluminium	7.5
nitrogen	3	iron	5
calcium	2	calcium	3.4
phosphor	1	sodium	2.6
K, S, Cl, Na,		hydrogen	0.8
Mg, Fe	0.9	Ti, Cl, P	0.6



# Carbon – natural occurrence 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 deposits – 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)

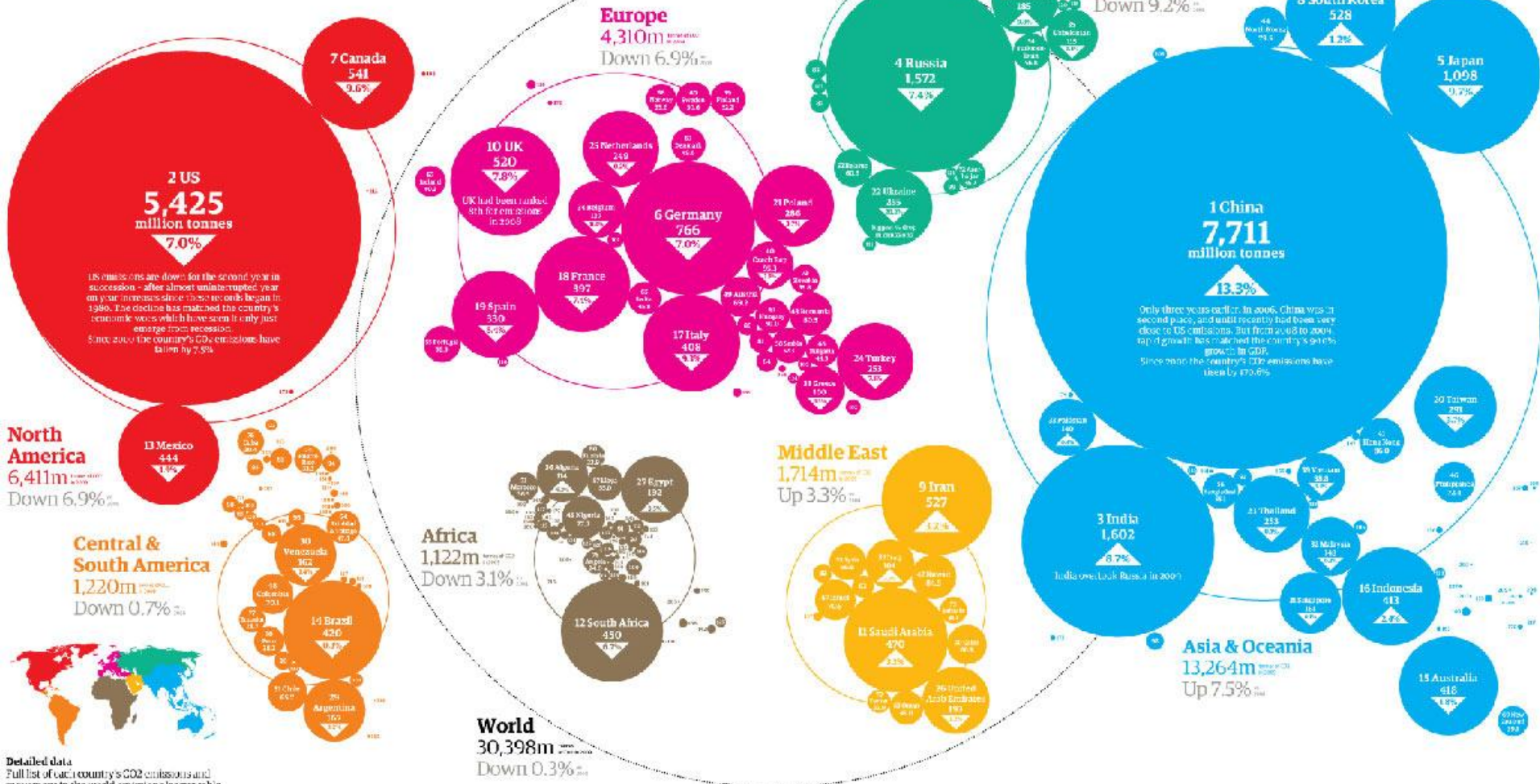




# An atlas of pollution: the world in carbon dioxide emissions

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 CO<sub>2</sub> emissions. And, for the first time, world emissions have gone down.

1.5% less  
7.2% more  
Decreases in emissions country  
Increases in CO<sub>2</sub> emissions 2009  
Data for 2009, 2010 & 2011  
Global emissions in 2009



**2 US**  
**5,425 million tonnes**  
7.0%  
US emissions are down for the second year in succession - after almost uninterrupted year on year increases since these records began in 1980. The decline has matched the country's remarkable boom which has seen it only just emerge from recession. Since 2005, the country's CO<sub>2</sub> emissions have fallen by 7.5%

**North America**  
**6,411m**  
Down 6.9%

**Central & South America**  
**1,220m**  
Down 0.7%

**Europe**  
**4,310m**  
Down 6.9%

**6 Germany**  
**766**  
7.0%

**10 UK**  
**520**  
7.8%

UK had been ranked 8th for emissions in 2008

**Africa**  
**1,122m**  
Down 3.1%

**12 South Africa**  
**450**  
4.2%

**Middle East**  
**1,714m**  
Up 3.3%

**9 Iran**  
**527**  
1.2%

**11 Saudi Arabia**  
**470**  
2.5%

**Eurasia**  
**2,358m**  
Down 9.2%

**1 China**  
**7,711 million tonnes**  
13.3%

Only three years earlier, in 2006, China was in second place, and until recently had been very close to US emissions. But from 2008 to 2009, rapid growth has allowed this country's series to overtake the US. Since then, the country's CO<sub>2</sub> emissions have risen by 173.6%

**5 Japan**  
**1,098**  
0.2%

**8 South Korea**  
**528**  
1.2%

**Asia & Oceania**  
**13,264m**  
Up 7.5%

**3 India**  
**1,602**  
8.7%

India overtook Russia in 2009

**15 Australia**  
**416**  
1.5%

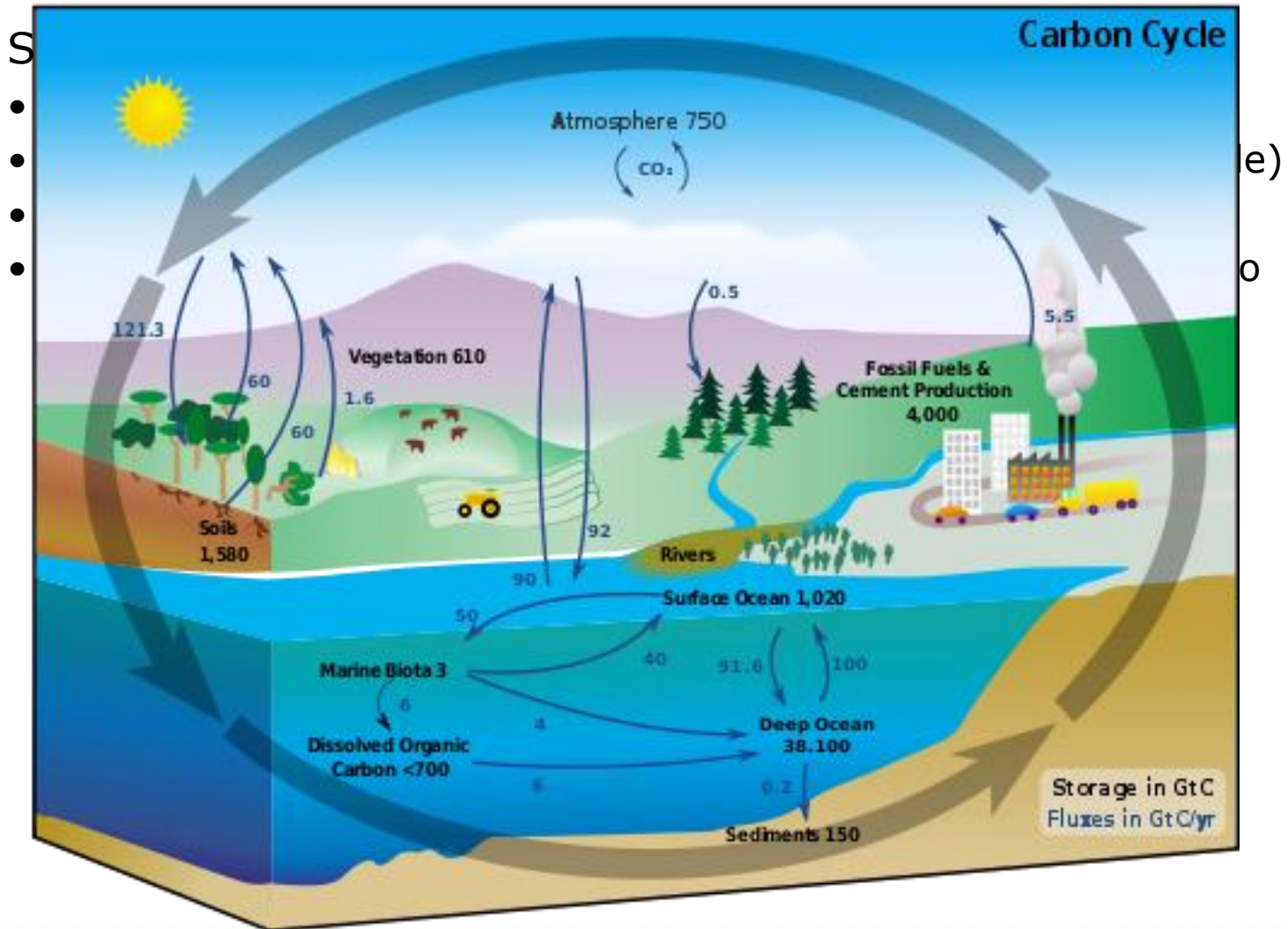
**World**  
**30,398m**  
Down 0.3%

Detailed data  
Full list of each country's CO<sub>2</sub> emissions and movement in the world emissions league table

Rank	Country	2009 Emissions (m tonnes)	% Change	Rank	Country	2009 Emissions (m tonnes)	% Change	Rank	Country	2009 Emissions (m tonnes)	% Change	Rank	Country	2009 Emissions (m tonnes)	% Change
1	China	5,425	13.3%	11	Canada	541	9.6%	21	Poland	326	0.2%	31	Belgium	185	0.1%
2	US	5,425	7.0%	12	South Africa	450	4.2%	22	UK	520	7.8%	32	France	397	2.5%
3	India	1,602	8.7%	13	Brazil	420	0.8%	23	Germany	766	7.0%	33	Spain	330	5.0%
4	Russia	1,572	7.4%	14	Argentina	167	0.7%	24	Italy	408	5.1%	34	Iran	527	1.2%
5	Japan	1,098	0.2%	15	South Korea	528	1.2%	25	France	397	2.5%	35	Saudi Arabia	470	2.5%
6	South Korea	528	1.2%	16	Indonesia	413	2.4%	26	UK	520	7.8%	36	Iran	527	1.2%
7	Canada	541	9.6%	17	Australia	416	1.5%	27	Poland	326	0.2%	37	Iran	527	1.2%
8	UK	520	7.8%	18	India	1,602	8.7%	28	Germany	766	7.0%	38	Iran	527	1.2%
9	Iran	527	1.2%	19	China	7,711	13.3%	29	Italy	408	5.1%	39	Iran	527	1.2%
10	UK	520	7.8%	20	Japan	1,098	0.2%	30	Spain	330	5.0%	40	Iran	527	1.2%

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# Carbon cycle

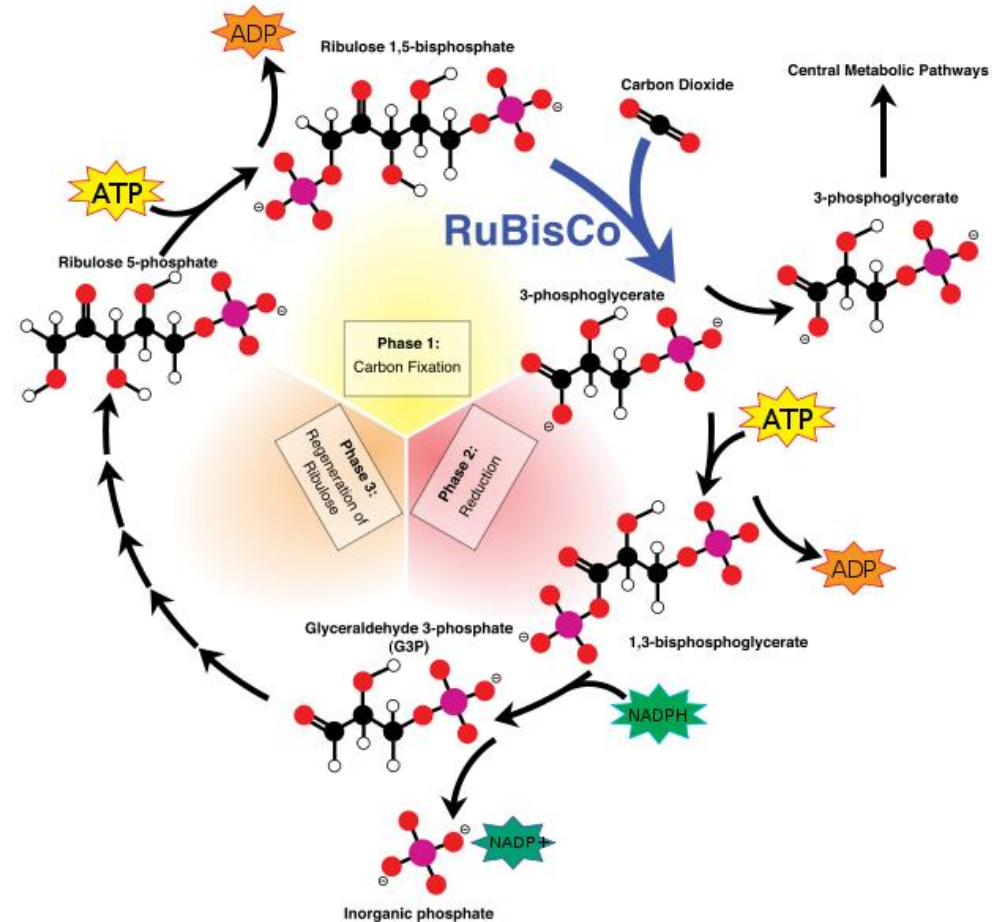




# Calvin Cycle

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 compound production from CO<sub>2</sub>



# 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

