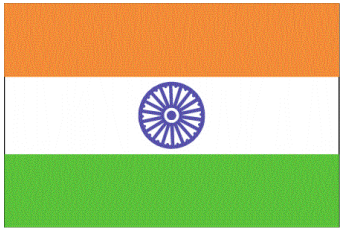
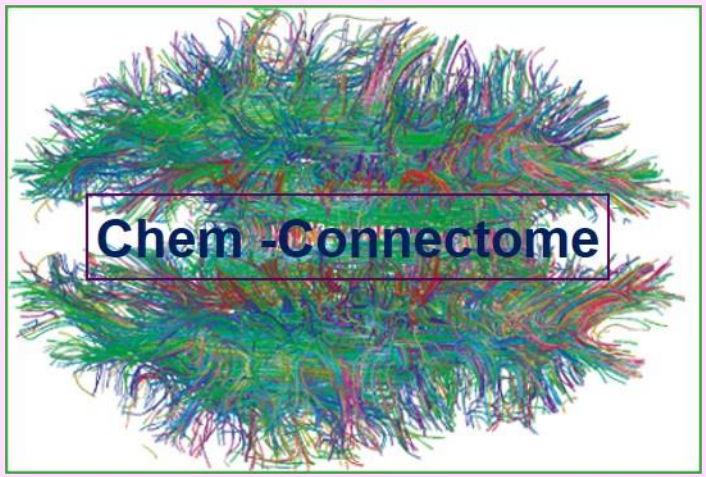
Dimensionality of Chemistry: A Science for Global Sustainability in the 21st Century



A grand safari of the chemical world……..

Contours of presentation

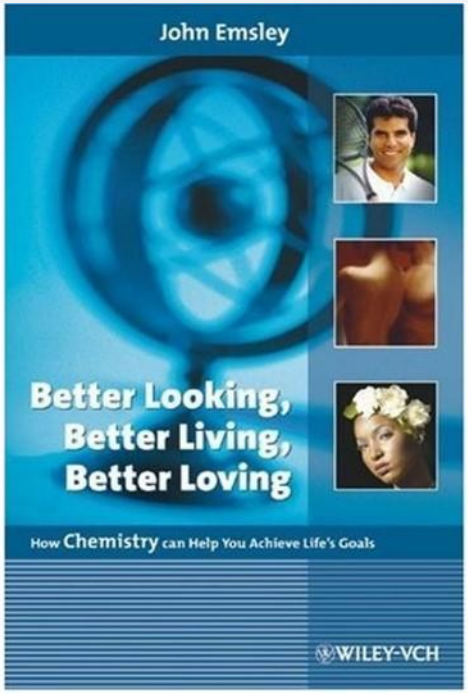
- Serenading chemistry - an omnipresent science
- Chemical science - art & craft of molecular creation
- The past as present and future – refreshing chemistry
- Glimpsing the horizon – chemistry as sustainability science



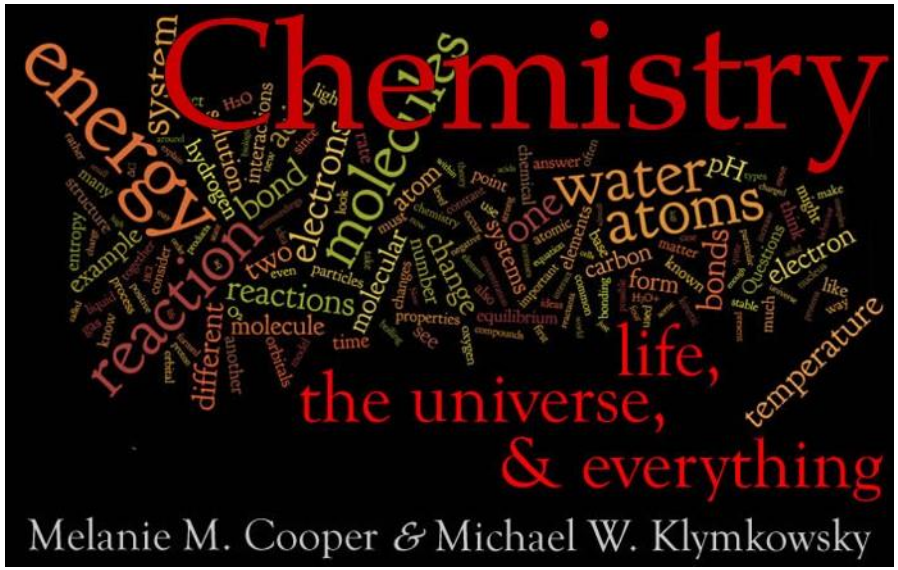
Disclaimer:

If you find this presentation provocative, think a bit more and responsibly for our future.

Chemistry is in everything and everything is in it, it is the basis of life, without it we wouldn't exist.



"How Chemistry can Help You Achieve Life's Goals"

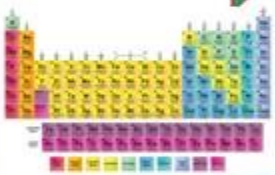


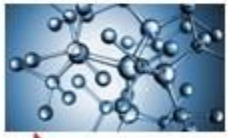
What in the world isn't chemistry? Evolving beyond the periodic Table!

"Chemistry Embraced by All"
S.A. Matlin, G. Mehta, H. Hopf*, Science*, **2015**, *347*, 1179

Chemistry – early moorings and the present

BCE





19th Century

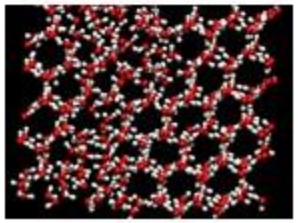
Art & craft of mixing substances

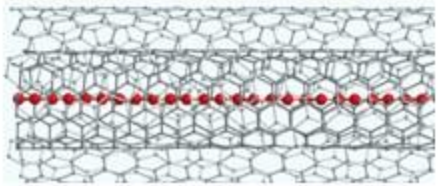
A giant knowledge leap

Alchemy to modern science

Discipline in a Table - systematization

'Molecularization' of chemical matter





The evolving perception of chemistry

19th Century

Value added products from almost anything and everything

"Utility science"

Molecular understanding of life processes and chemical matter

"Core Science"

Interdisciplinarity in forefront

"Integrative Science"

Resource stressed planet

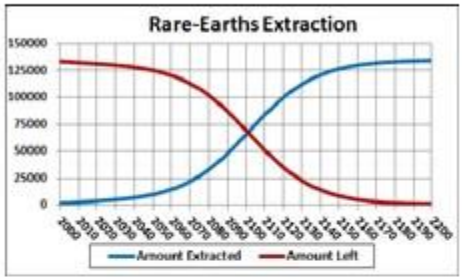
"Sustainability Science"

21st Century

S. A. Matlin, G. Mehta, H. Hopf, A. Krief. *Nature Chemistry* **2015**, *7(12)*, 941-943

The evolving perception of chemistry

19th Century



Estimate: By 2050 - 180 Bn tones p.a. of natural resources will be needed. (currently 90 Bn p.a.)
This is unsustainable!

Chemistry can pave the way: Greener, leaner, resource prudent, efficient processing, **recycling**…

Rapid depletion of lithium and rare earths

CO_2 <400 ppm

Resource stressed planet

"Sustainability Science"

21st Century

S. A. Matlin, G. Mehta, H. Hopf, A. Krief. *Nature Chemistry* **2015**, *7(12)*, 941-943

Chemistry prophecies and traits

'Study the past, if you would define the future' - Confucius

'Nothing is lost, nothing is created, everything is transformed'

- Antoine Lavoisier

'die chemie ist also die Lehre von den stofflichen metamorhosen der materie'

- A Kekulé

'Green' is in the DNA of Chemistry

Wohler
1827

'Ammonium cyanate is urea'

Green Synthesis

$NH_4Cl + AgNCO \longrightarrow [\,NH_4NCO\,] \rightleftharpoons H_2N{-}C(=O){-}NH_2$

100% Atom conservancy

CH_4N_2O $\qquad$ CH_4N_2O

Antoine Lavoisier
1743-1794

Humphry Davy
1778-1829

Jacob Berzelius
1779-1848

Michael Faraday
1791-1867

Friedrich Wohler
1800-1882

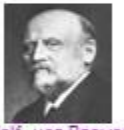
Justus von Liebig
1803-1873

Marcellin Berthelot
1827-1907

Augustus Kekule
1829-1886

Dmitri Mendeleev
1834-1907

Alfred Werner
1866-1919



Adolf von Baeyer
1835-1917

Wilhelm Oswald
1853-1932

Victor Grignard
1871-1935

G. N. Lewis
1875-1946

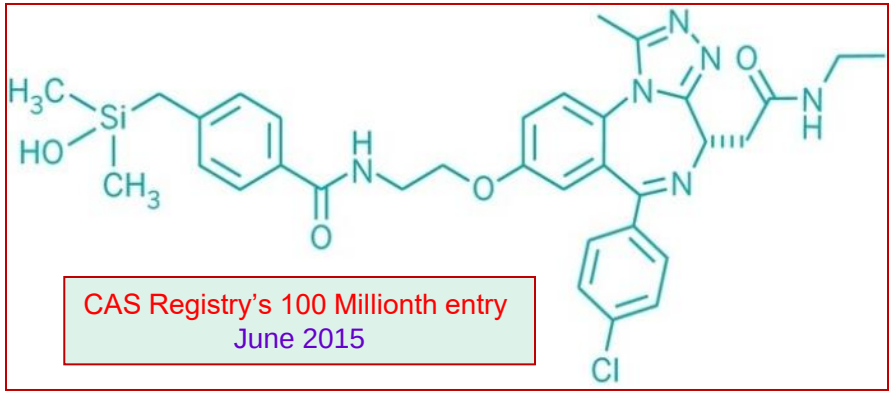
Molecular level view of everything and molecular creation is central to chemistry

Sizing the molecular cosmos

10^{80} to 10^{200} unique chemical structures possible

That is not far from infinity; impractical?

…and there is not enough mass in the Universe !



CAS Registry's 100 Millionth entry
June 2015

A galloping pace..
125 M in CA Registry, Dec. 2016;
many millions buried in patents;
best estimate ~ 0.5 billion NME's

Chemistry is also the science of the possible

Scope relevant chemical space

Mantra to remember…

Make only what is needed for human advancement and well-being;

in risk free, non-hazardous way with minimal environmental footprint.

Chemists are not merely molecular ‘cooks’

Is chemistry at the cross roads?

As a mature discipline, chemistry seems to have plateaued and trudges along as an incremental science without articulating big ambitions or addressing global challenges?

Let chemistry not recede to be a service science - a scientific equivalent of Latin - ***something you learn before you learn something else****."*

- Is there an erosion of its sheen and appeal?
- Can it deliver and survive in the business as usual mode?
- Does our science need re-invention and repositioning?

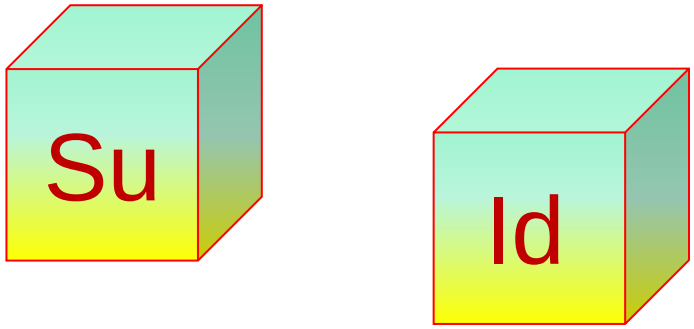
Chemistry needs re-invention and repositioning

Chemists must ponder ways to re-energize and refresh the discipline to render it 'fit-for-purpose' to meet the challenges of the 21st century

Chemistry will be the key enabler for providing clean energy, water, food, healthcare, shelter to worlds billions

To deliver on it, chemistry needs……

New symbols - Beyond the Periodic Table……

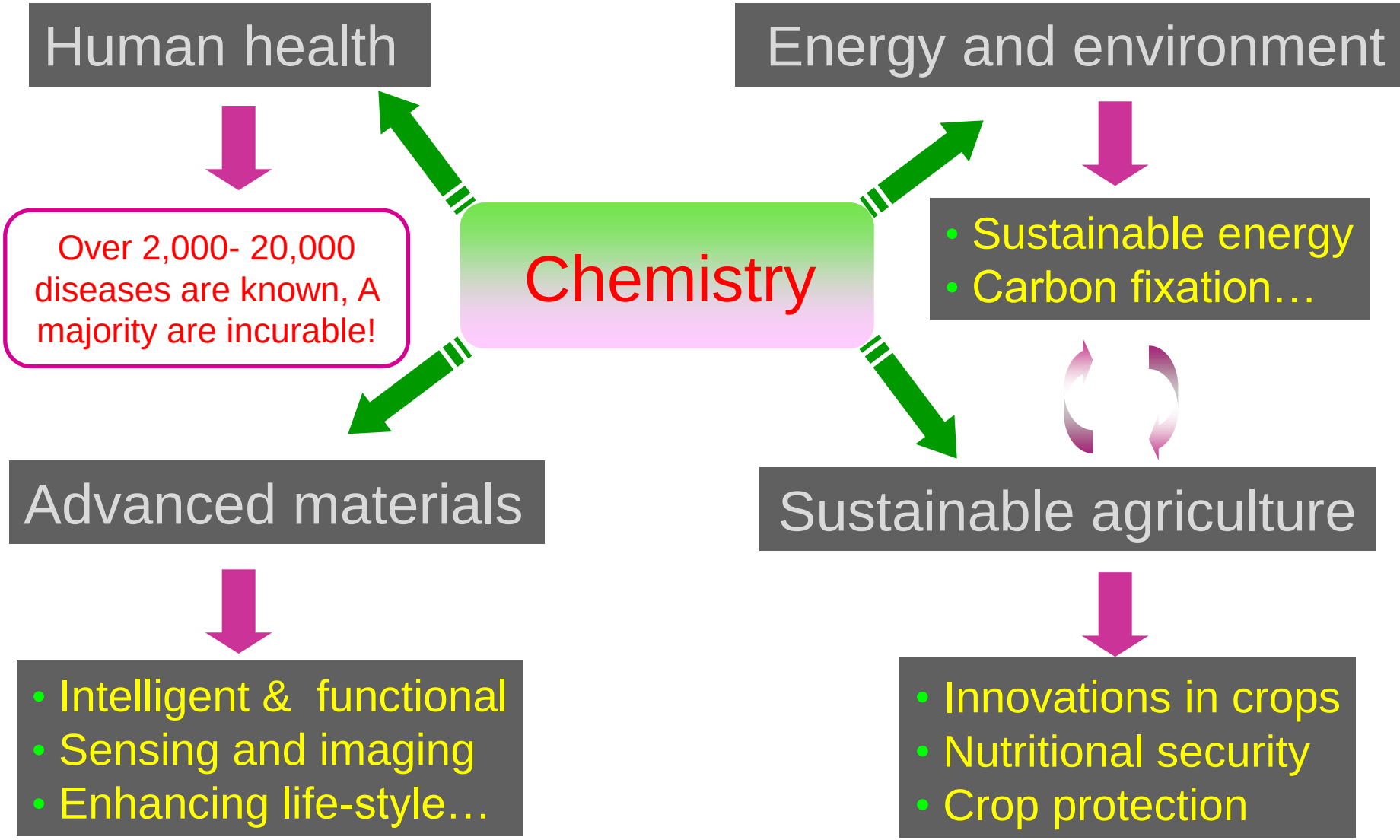


Retuning attitudes and mind-set

- Big picture: Identify mega challenges that capture public imagination,
  e.g. LIGO or CERN or Human Genome (from read out to writing?)……
- Collaborate, collaborate, collaborate; forge large networks-
  Across disciplines and geographies (PACN-RSC, FACS, EuChemMS?)
- Resist the 'rearranging the deck chairs on the Titanic' affliction,
  Beyond one's methodology, process, technique, reaction, catalyst, algorithm….

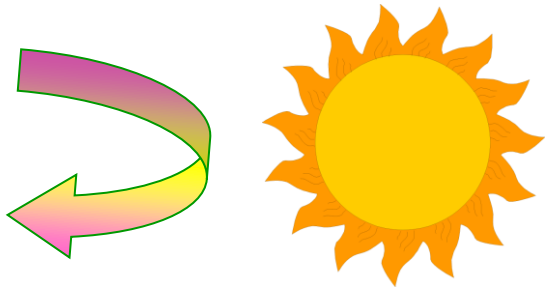
New opportunities, challenges and promises to keep;
Chemistry can!

Opportunities……on path to sustainability



Sustainable Energy and Environment

Powering the planet: Sun pours more energy on to the earth's surface in an hour than the planet uses in a year!



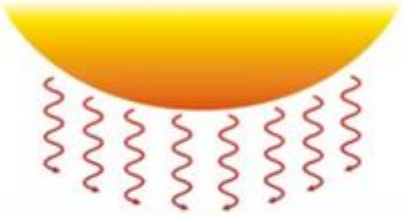
- Solar - PV, Solar-thermal
- Renewable - Biomass
- Water Splitting – H_2

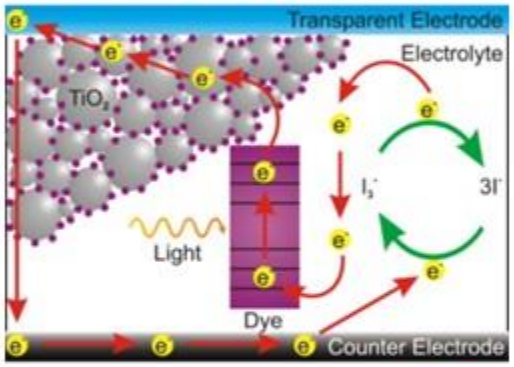
- CO_2 fixation & recycling
- CO_2 sequestration

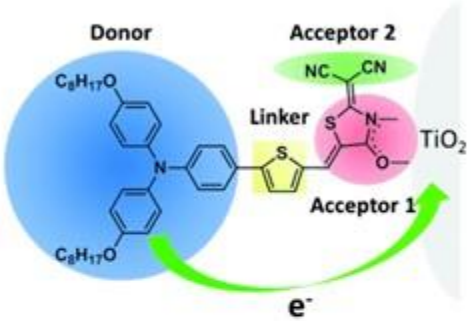
Sustainable Energy and Environment

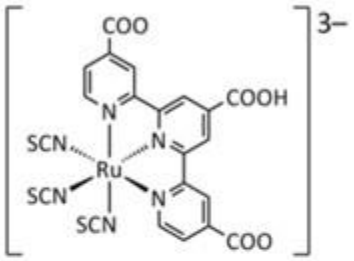
Organo-electronics

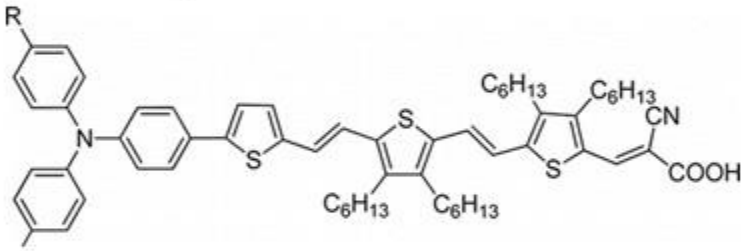
Vacuum-moulding graphene into nano-corduroy

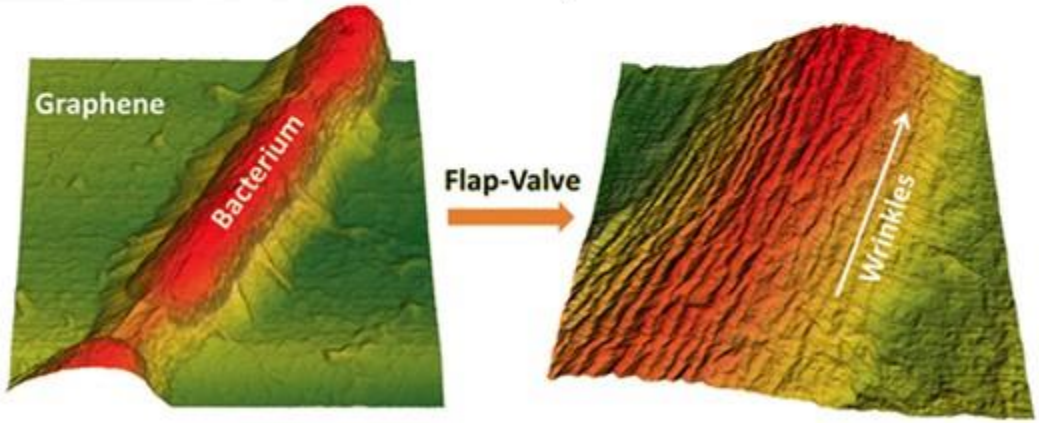












Unlocking electronics potential!

ACS Nano **2016** asap; **DOI:** 10.1021/acsnano.6b03214

Sustainable Energy and Environment

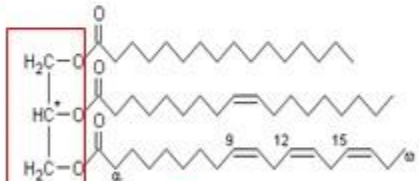
- Solar – PV, Solar-thermal
- Renewable - Biomass
- Water Splitting – H_2

- CO_2 Sequestration
- CO_2 Fixation & recycling

Harness Nature's photosynthesis machinery

Blue green Algae: photosynthetic power cell

Algae based biofuels



Biodiesel

Glycerol

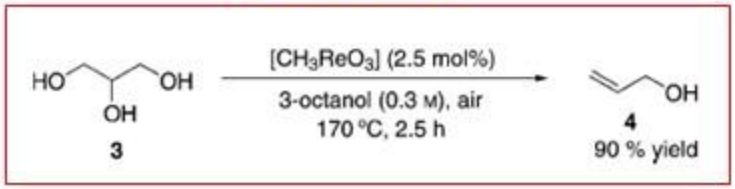
Cat.

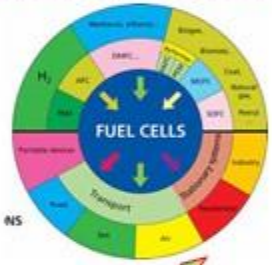
CH_3OH

Catalyst

Hydrocarbons

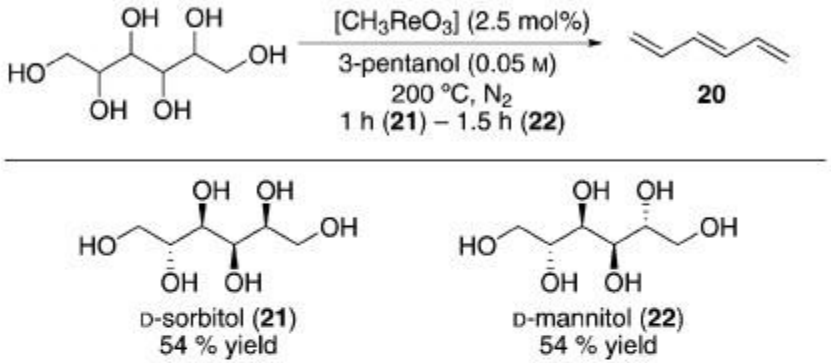
Valorization





energy and environment

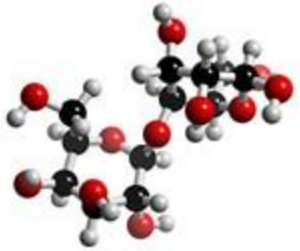
Cellulosic waste to hydrocarbons

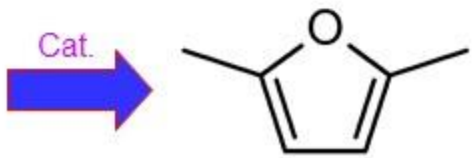


Shiramizu & Dean Toste, *Angew Chem.* **2012**, *51*, 8012

Depolymerization of cellulose using solid catalysts in ionic liquids - biofuel

F. Schuth et al. Angew. Chem. Intl. Ed. 2008





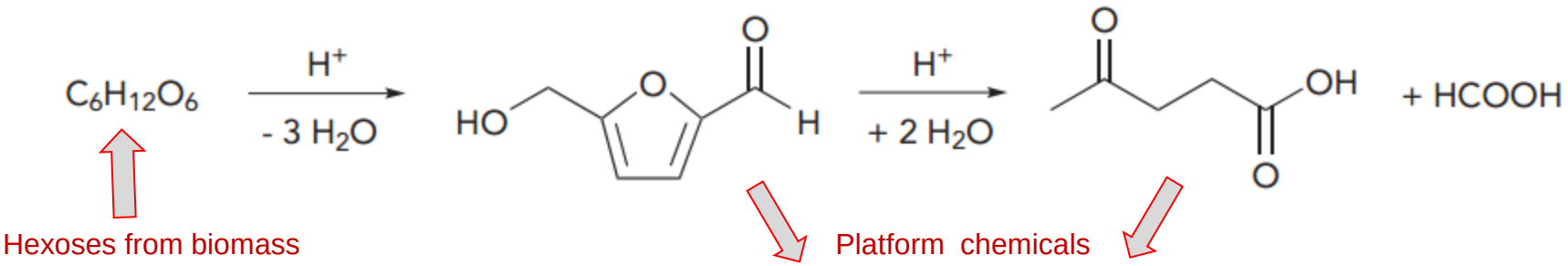
"Stripping oxygens"

2,5-dimethylfuran (DMF) as biofuel

J. Dumesic *et al. Nature*, **2008**

Challenge:

Catalytic up-gradation of bio-derived feed stocks while minimizing the loss of carbon and the generation of by-products, particularly CO_2.

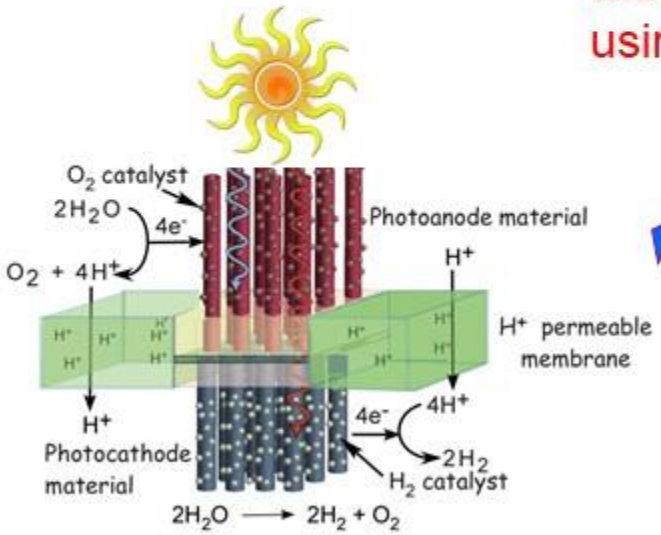


Review: Dean Toste *et al. Chem* **2016**,*1*, 32.

Water as a fuel!

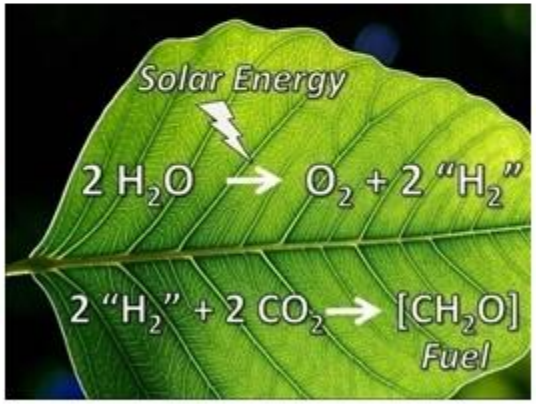
Use of Sunlight to split water or artificial photosynthesis is the Holy Grail of renewable energy research

Arrays of microwires coated with catalysts to split water using sunlight to make H_2.



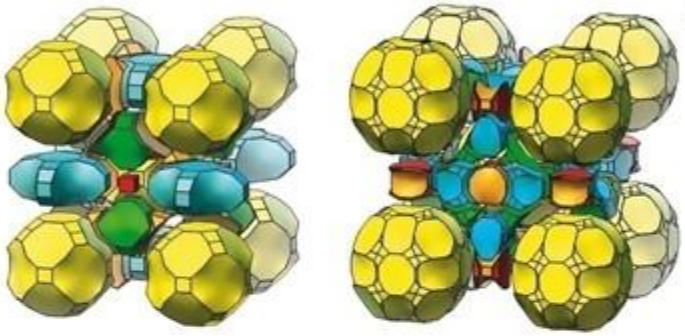
A practical artificial leaf has been devised

D. Nocera *et al.*



Energy and Environment - CO_2 Sequestration

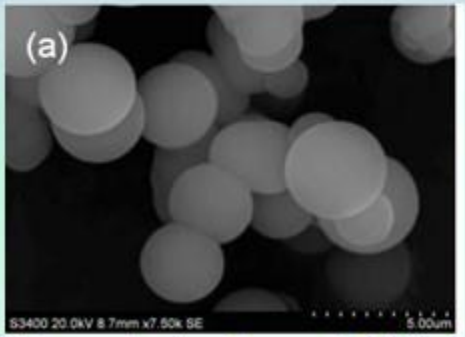
CO_2 capture: Colossal cages in zeolitic imidazolate (ZIF) frameworks as selective carbon dioxide reservoirs



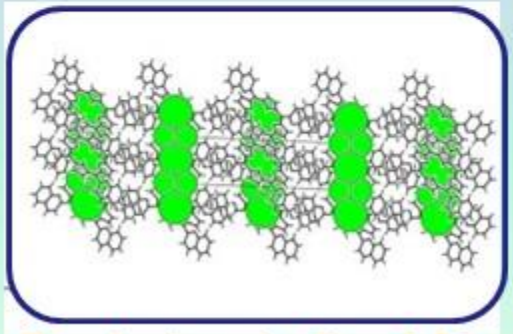
ZIF's have complex cages, up to 264 vertices, and as many as 7,524 atoms that can store ~100 times CO_2

Yaghi *et al. Nature* 453, **2008**, 207

CO_2 Capture: Polymeric organic frameworks (POF)

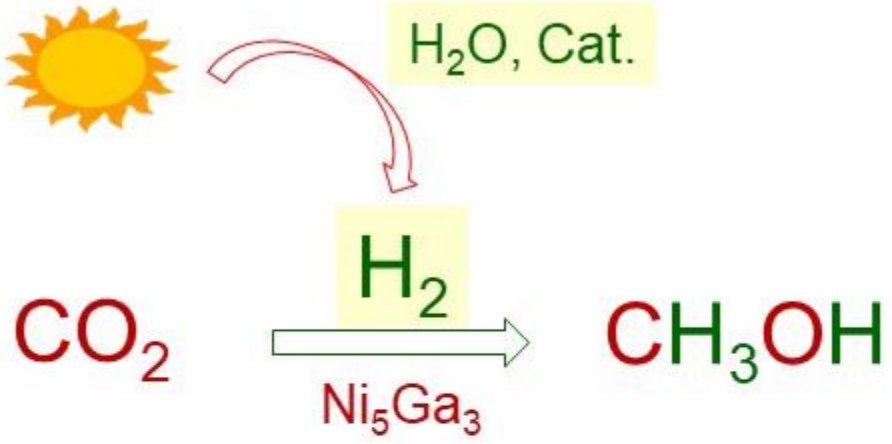


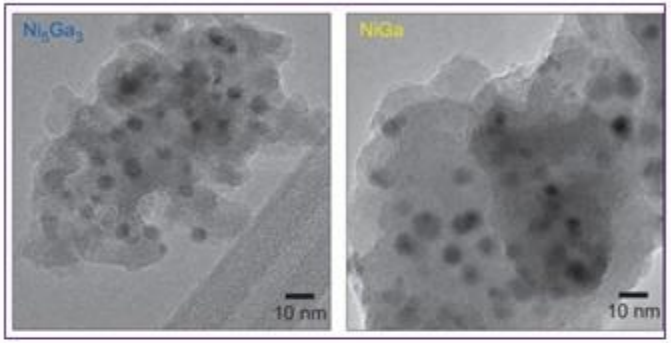
Phloroglucinol based; 18% CO_2



Porphyrin-quinoline; 1-5 bar

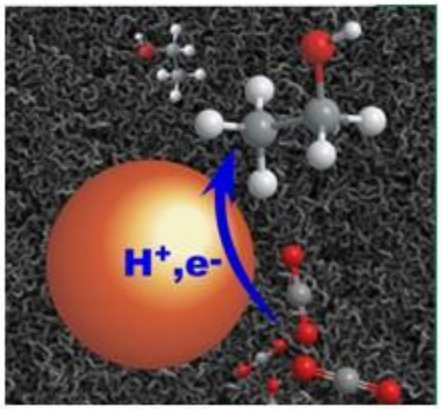
Towards carbon dioxide fixation





F. Studt *et al. Nature Chemistry*, 2014, doi:10.1038/nchem.1873

Euraka moment! Electrochemical reduction of CO_2 to ethanol



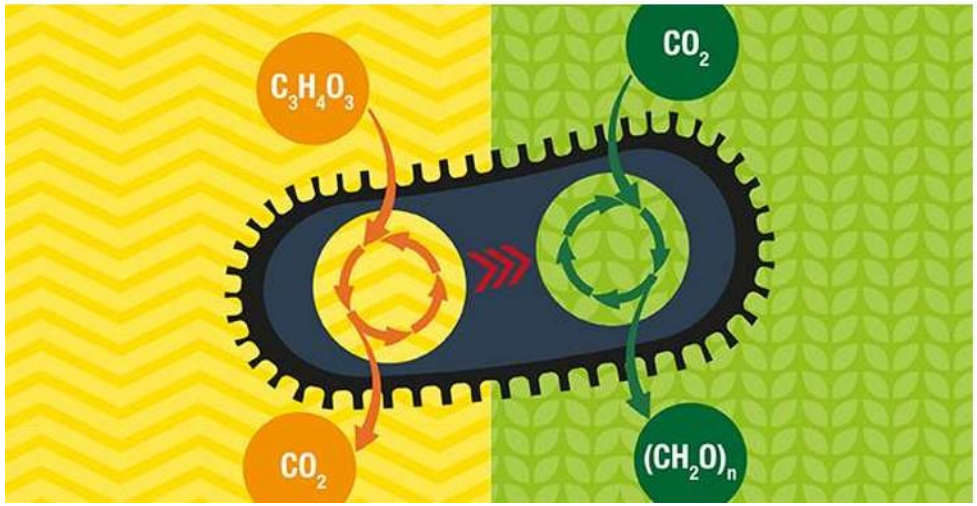
$$2\ CO_2 + 9\ H_2O + 12\ e^- \rightarrow C_2H_5OH + 12\ OH^-$$

Copper nanoparticle/N-doped Graphene electrode

Song *et al.* ChemistrySelect **2016**, *1*, 6055

Towards carbon dioxide fixation

Biochemical fixation: Sugar Synthesis from CO_2 in *Escherichia coli*



Reprogramming organisms
(inserting Calvin cycle components into *E. coli*

Antobosky *et al. Cell* **2016**,*166*, 115-25.

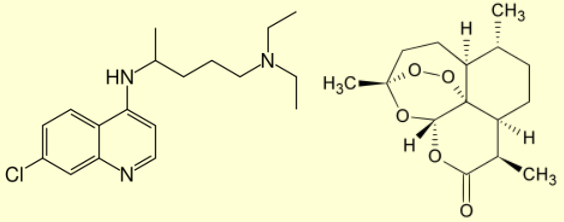
Chemisty for human health and well-being

Human health & wellbeing

Drugs for emerging and resistant diseases, modulation of cognitive functions and interpersonal behavior……..

On average antibiotics add 20 years to each person's life

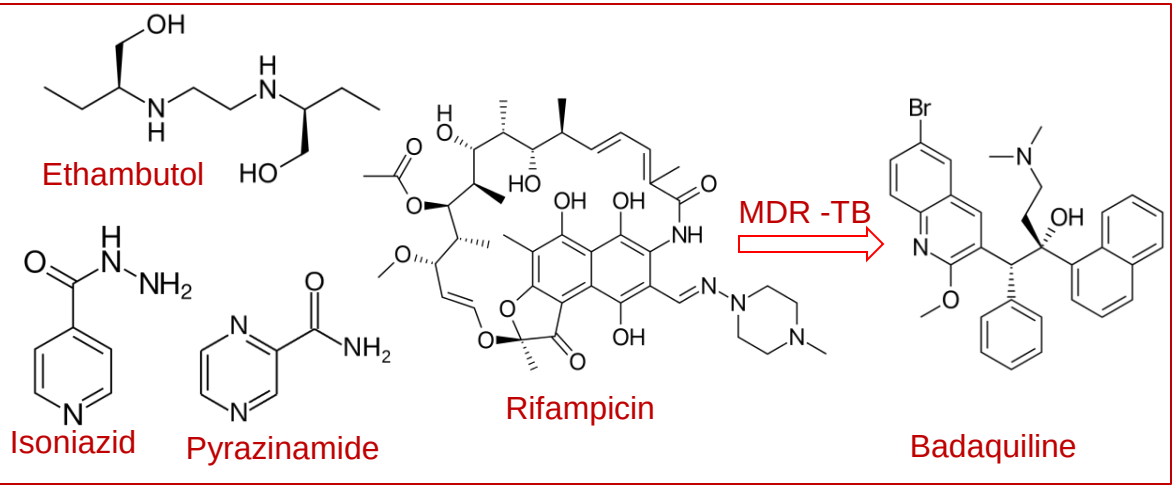
Eradicating malaria?



From Chloroquine to Artemisinin

Mortality rate of 1.2 million per year

Fight against tuberculosis

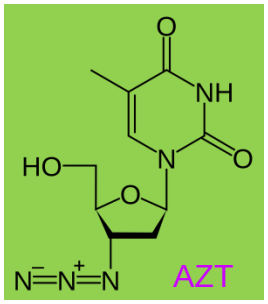


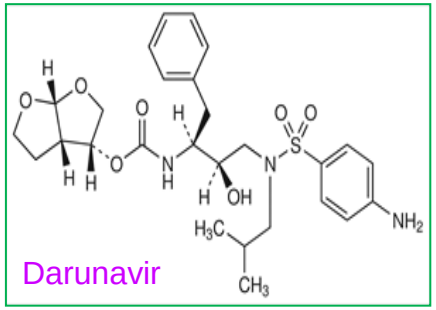
Human health & wellbeing

Drugs for emerging and resistant diseases, modulation of cognitive functions and interpersonal behavior……..

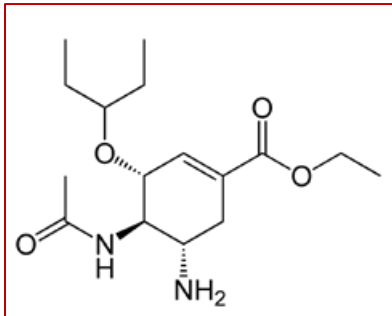
On average antibiotics add 20 years to each person's life

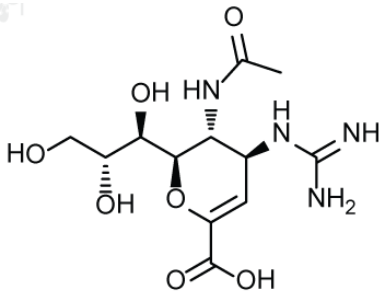
Anti-AIDS Cocktail

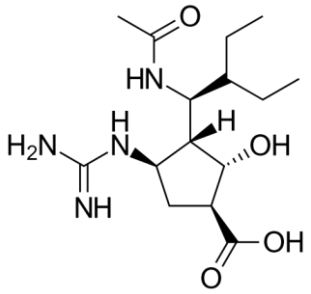




Battling 'avian flu'

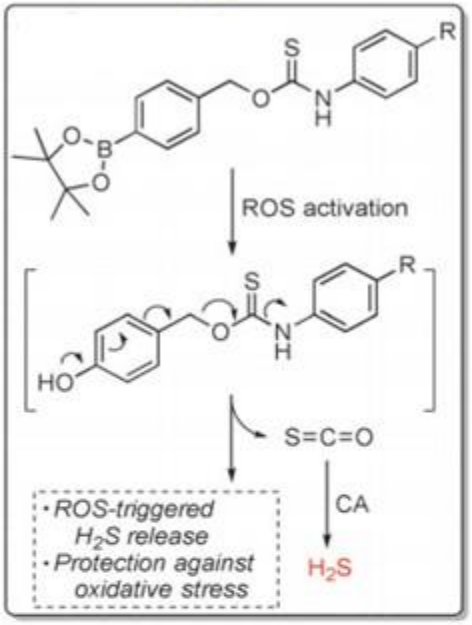


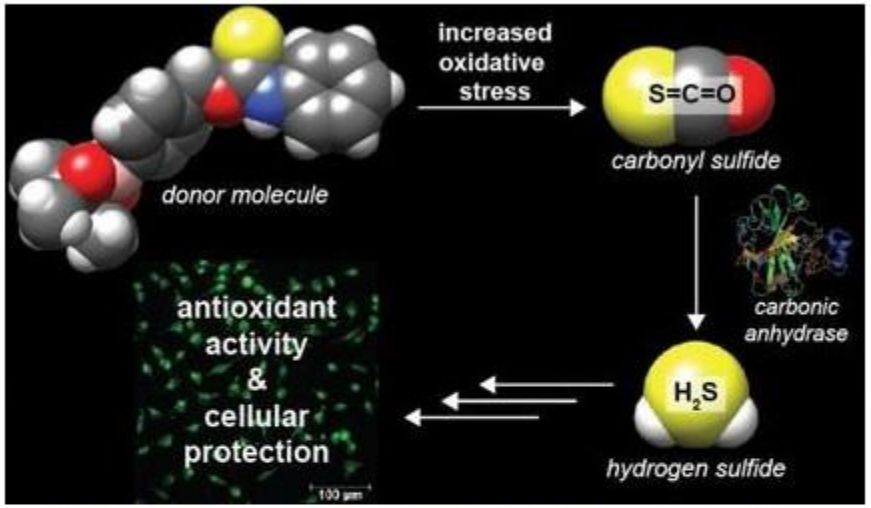




Impressive responses to recent pandemics like Zica and Ebola

H_2S for stressed cell recovery- on site delivery?





Pluth *et al. Angew. Chem. Int. Ed.* **2016**, *55*, 14638

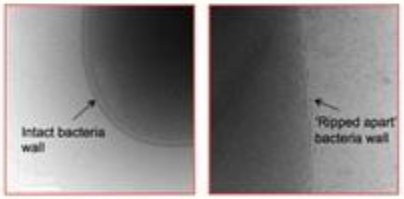
Organic molecules that release hydrogen sulfide under certain biological conditions like oxidative stress, and may protect cells.

Beyond antibiotics: A major global health challenge

'Superbugs' are projected to kill 10 M people by 2050

Peptide chains in Star like shape

Combating multidrug-resistant Gram-negative bacteria with nano-engineered antimicrobial peptide polymers.



Bacterial wall before (L) and after (R) exposure to star shaped polymer

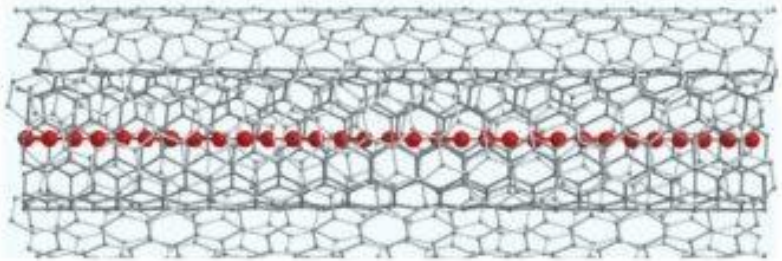
G. Jiao *et al. Nature Microbiology*; doi:10.1038/nmicrobiol.2016.162

A collage of smart, intelligent materials

Shape memory & stimuli-responsive materials

"smart" materials that will allow the wings of a craft to change shape for optimal flying conditions.

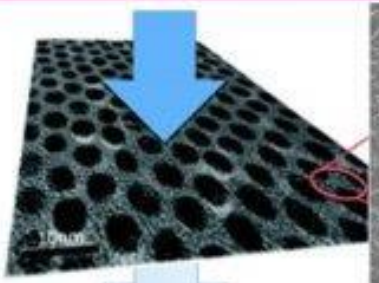
Polymers with dynamic "shape memory": On thermal/ electric/ light stimuli shape memory polymers exhibit reversible change from rigid polymer to elastic state.

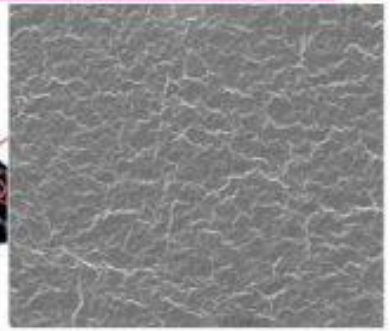


'Carbyne'
40 times harder than diamond

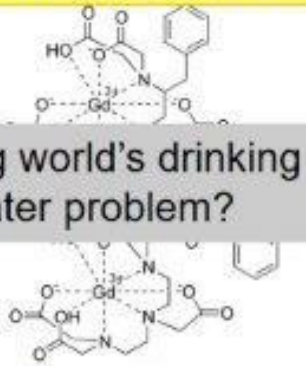
Thinnest nanof

Large-area graphene-oxide membranes





Solving world's drinking water problem?



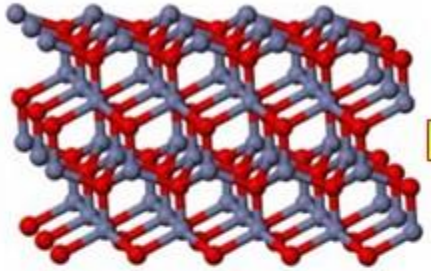
30 nm thick; rejects

Nat. Commun. doi: 10.1038/ncomms10891 (2016).

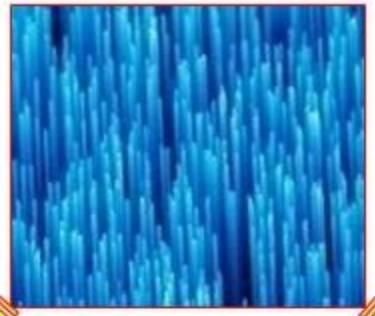
Imaging

Pulmonary angiography

Sensing wonders at *atto*- and 0.00000000000000000001 M



ZnO



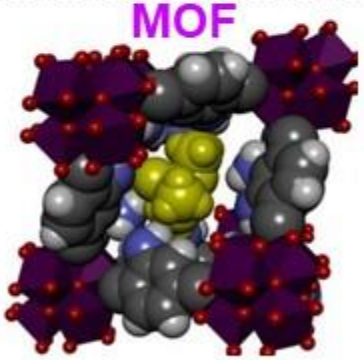
ZnO nano-wires

New architectures for sensing, imaging, memory storage, optical communications & – CHEMICAL SENSING

10-50 nm diameter - 20,000 could fit in the eye of a full-sized needle

one-thousandth the diameter of a human hair

MOF



Artificial Nose – Smell Receptor

- To detect diseases like cancer, malaria..
- To sniff chemicals, poisons, explosives…
- To sequester and separate gases

'NaNose' can sniff VOC to detect lung cancer with 90% accuracy, *June, 2016*

Chemistry as an ethical science

May 2016

- ACS has created a Global Code of Ethics (GCCE) for chemists based on the Hague Ethical Guidelines*;
- GCCE is aspirational and encourages responsible practice of chemistry and makes a strong pitch for environment and sustainability;
- Expands beyond the traditional concerns about personal conduct & practice of collegiality, research integrity and transparency;
- Ethics education to be integral part of chemistry education.

* https://www.acs.org/content/acs/en/education/students/graduate/gettingready/ethics.html

Chemistry will be the ‘fundamental science’ in quest for sustainability in the 21st Century

Concluding thoughts

- Harness the omnipresence of chemistry as science for everybody.
- Recognize the role of chemistry in inventing a sustainable future.
- Reposition from ‘being a science’ to ‘being a science for the benefit of society’
- Adopt the concept of ‘one-world chemistry and systems thinking’

www.**oneworldchemistry**.org

S.A. Matlin, G. Mehta, H. Hopf*, Science*, 2015, *347*, 1179

S. A. Matlin, G. Mehta, H. Hopf, A. Krief*. Nature Chemistry* **2015***, 7(12)*, 941

S. A. Matlin, G. Mehta, H. Hopf and A. Krief*, Nature Chemistry*, **2016**, *8*, 393

A. Palermo*. ‘The future of chemical Sciences’ Royal Society of Chemistry Report.* ***2016***

Thank you for your kind attention

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