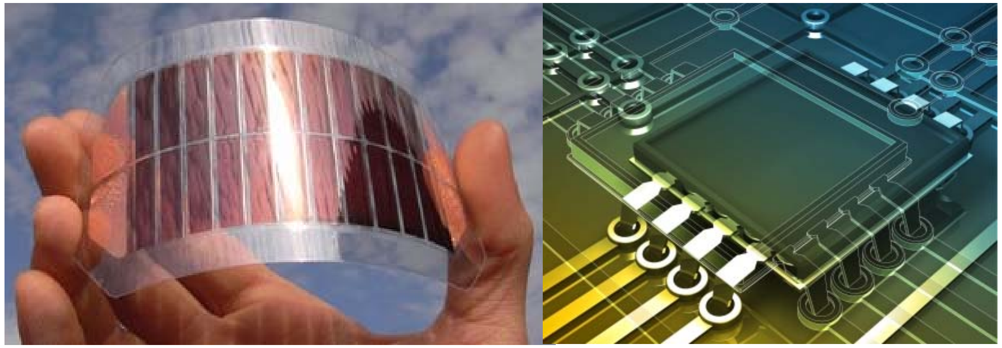
SpringerMaterials: Sample Researcher Use Cases

The SpringerMaterials Team

SpringerMaterials: Sample Researcher Use Cases

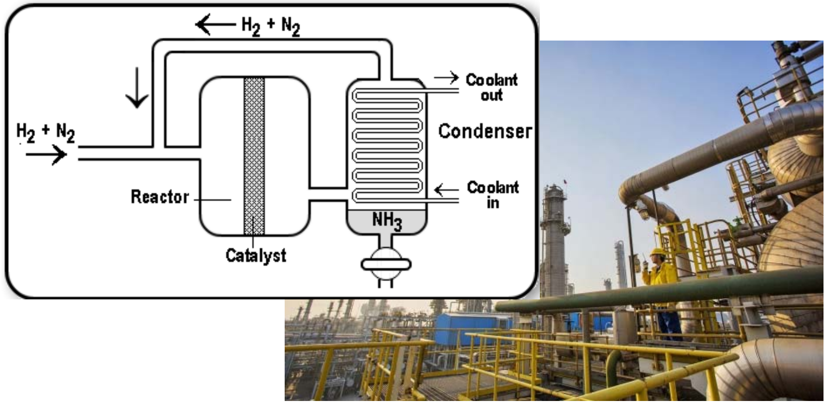
- Use Cases are presented for the three areas that SpringerMaterials is especially strong in
- Topics apply to academic/government and corporate research

Semiconductors & Electronics (3)



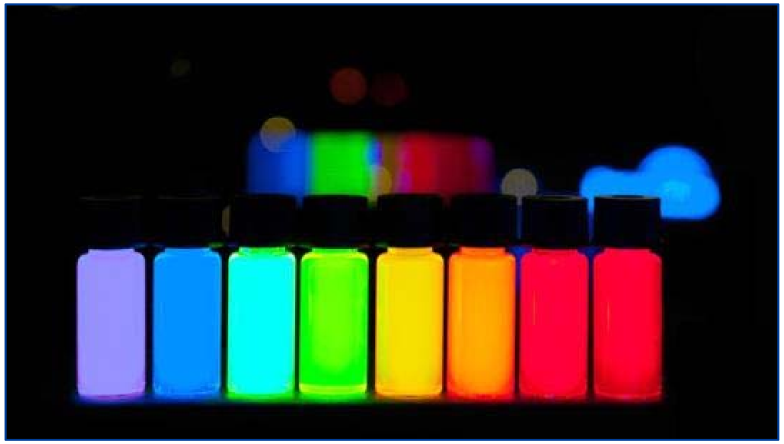
Metals, Alloys, Ceramics (3)

Chemical Processing & Energy Applications (4)



Semiconductors & Electronics: Quantum Dots

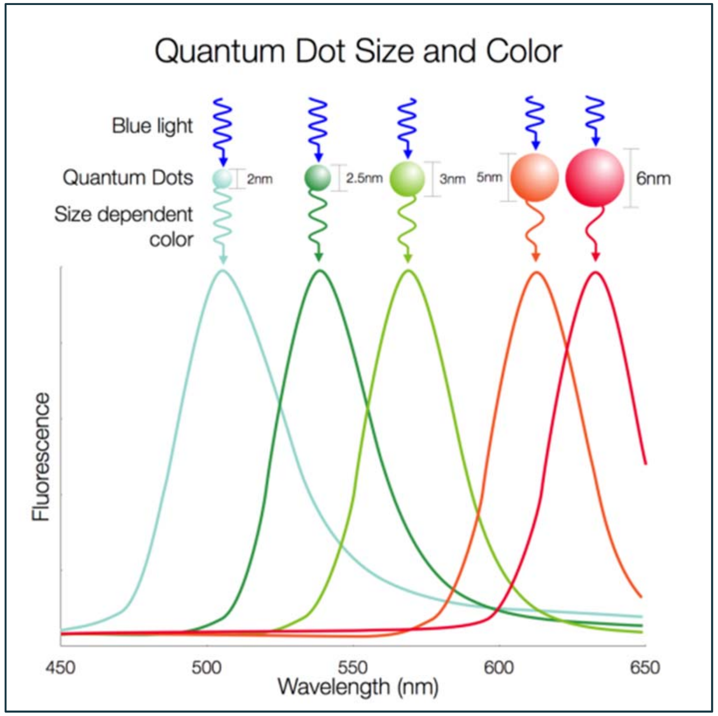
- **Quantum Dots** are semiconducting nanocrystals
- Nanocrystal size determines the color of emitted light
- Optical properties of quantum dots makes them attractive in **display devices**; **wider color gamut** and **richer colors**
- Quantum dot based devices are **now entering the market**:



plasmachem.com/shop/en/226-zncdses-alloyed-quantum-dots

LG G4 Quantum Display *(top)*
vs.
LG G3 (normal LCD) *(bottom)*

www.pocket-lint.com/news/133728-lg-g4-ips-quantum-display-explained-how-is-it-different-to-a-normal-lcd

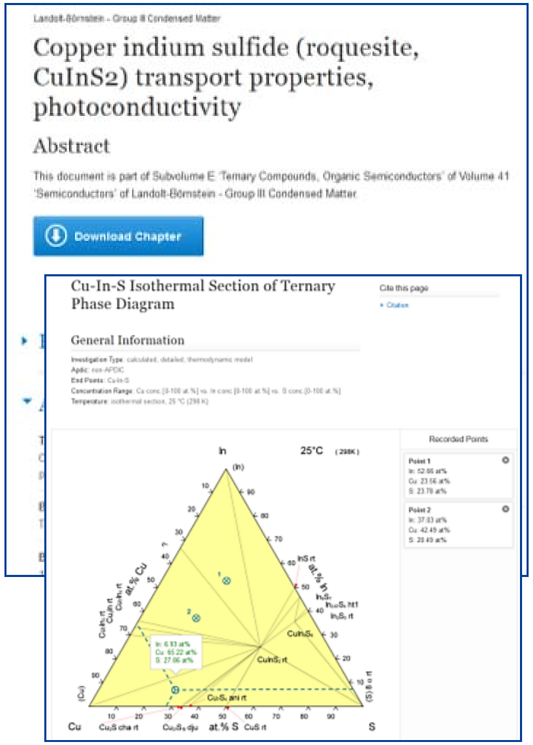


nanosysinc.com/what-we-do/quantum-dots/

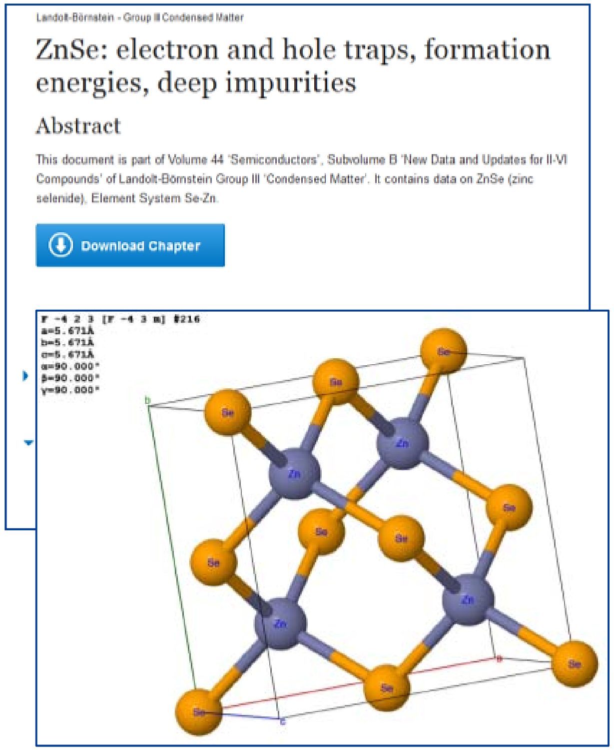
Semiconductors & Electronics: Quantum Dots

- Quantum dots traditionally use toxic heavy metals (Cd, Pb, or Hg)
- Use of these metals in consumer electronic devices is being strictly regulated (EU Directive 2011/65/EU); Cd/Pb/Hg-free quantum dots are of increasing interest
- SpringerMaterials contains detailed data on the preparation, characterization, and properties of many Cd/Pb/Hg-free quantum dots such as:

$CuInS_2$:



ZnSe:



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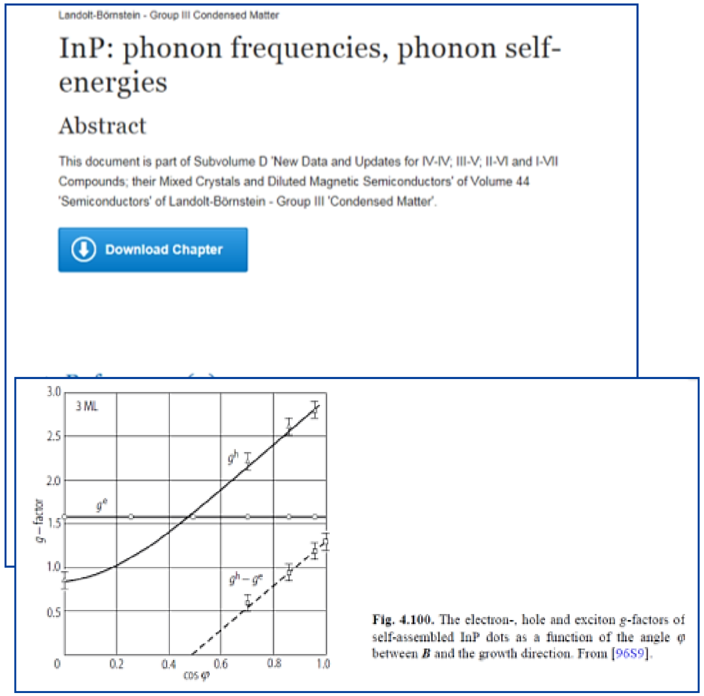
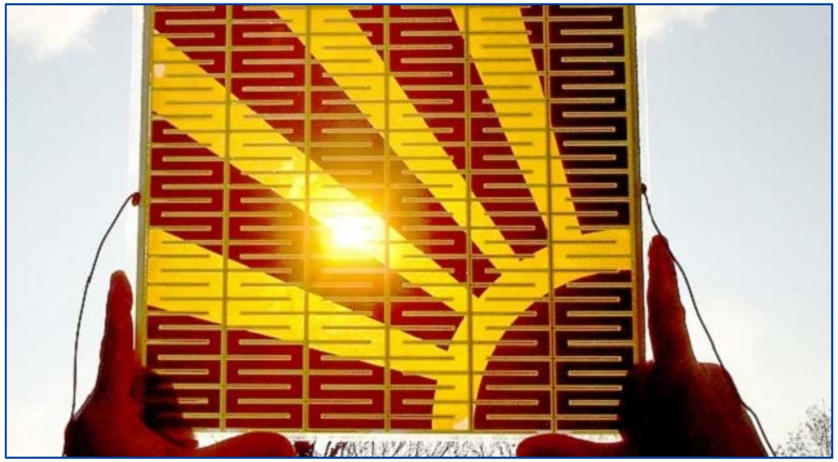


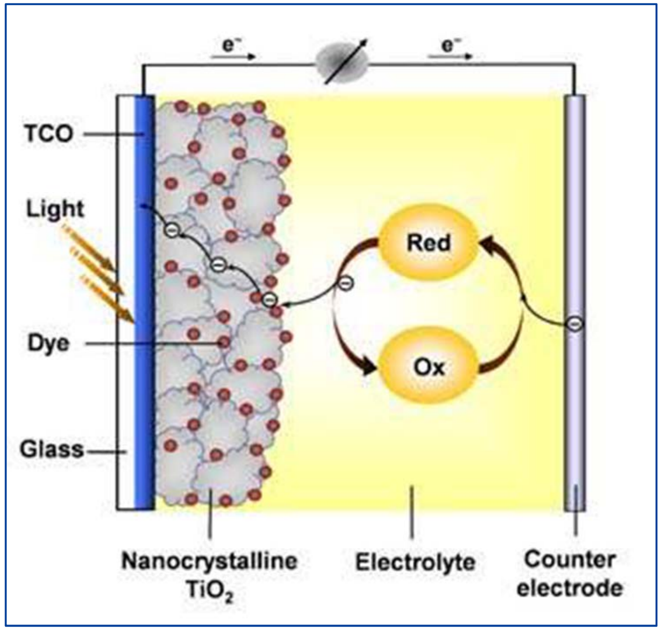
Semiconductors & Electronics: Dye Sensitized Solar Cells (DSSCs)

- **Dye sensitized solar cells** use organometallic dyes, semiconducting nanoparticles, and electrolytes to produce an electrical current
- DSSCs are **cheaper** than traditional Si-based cells, and **work well** even at **higher temperatures** and **low-light** (indoor) conditions
- Major applications include "**solar cell windows**":



borderstep.org/projects/sustainable-product-innovation-using-dye-sensitized-solar-cells/

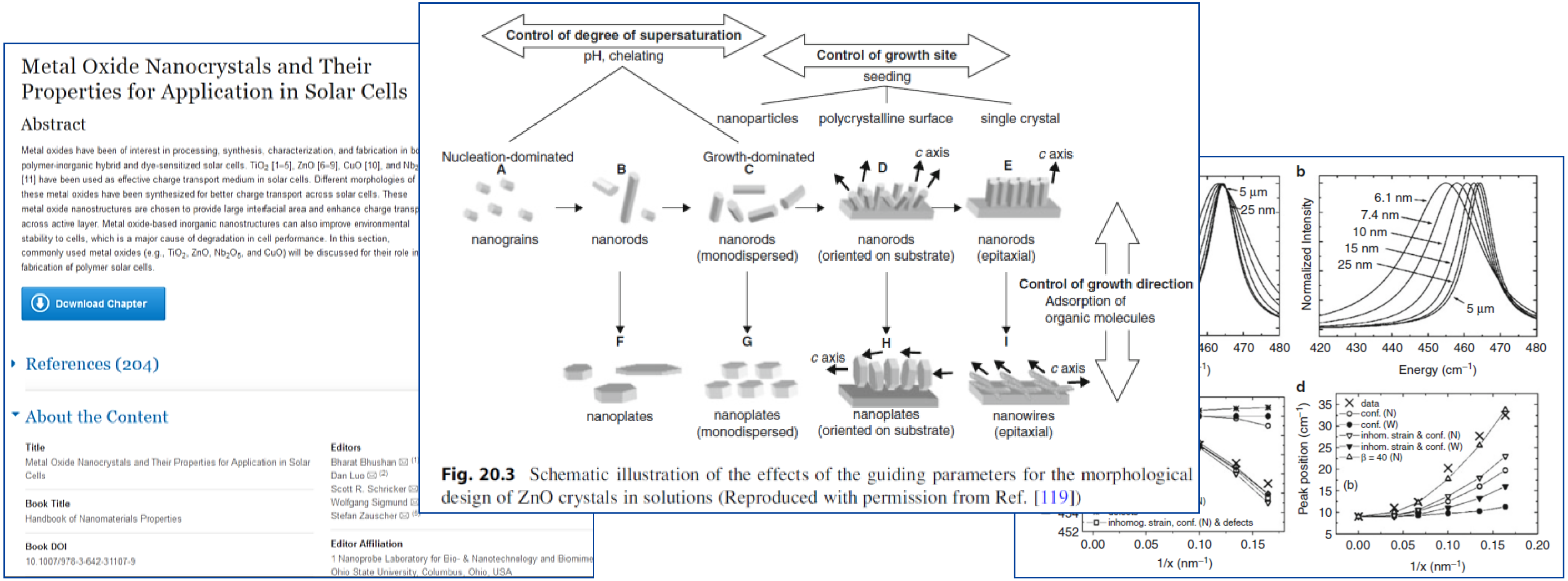
Western façade of the SwissTech Convention Center (Lausanne) covered in DSSCs



people.bath.ac.uk/pysabw/abwmod.html

Semiconductors & Electronics: Dye Sensitized Solar Cells (DSSCs)

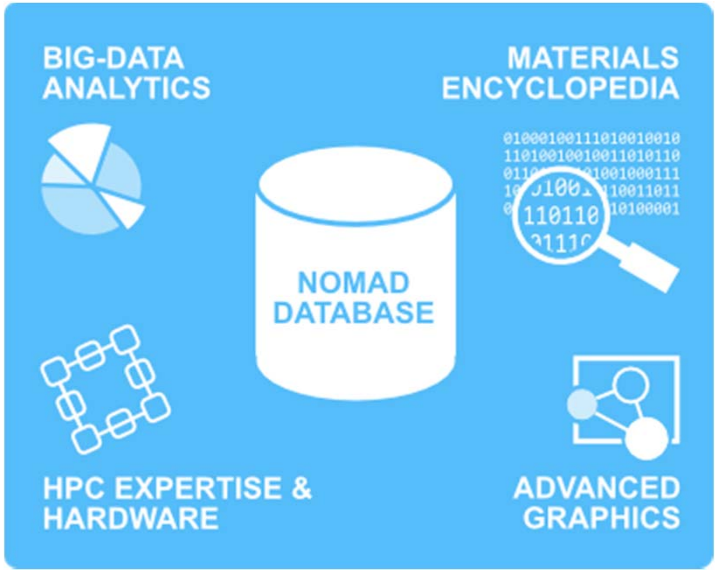
- Early DSSCs used liquid electrolytes; low efficiencies, limited operating temperatures, and hazardous solvents
- Solid state electrolytes have revolutionized the field; power conversion efficiencies of up to 15% (among the highest)[1]
- SpringerMaterials has extensive information on solid state materials relevant for modern DSSCs (e.g., metal oxides):

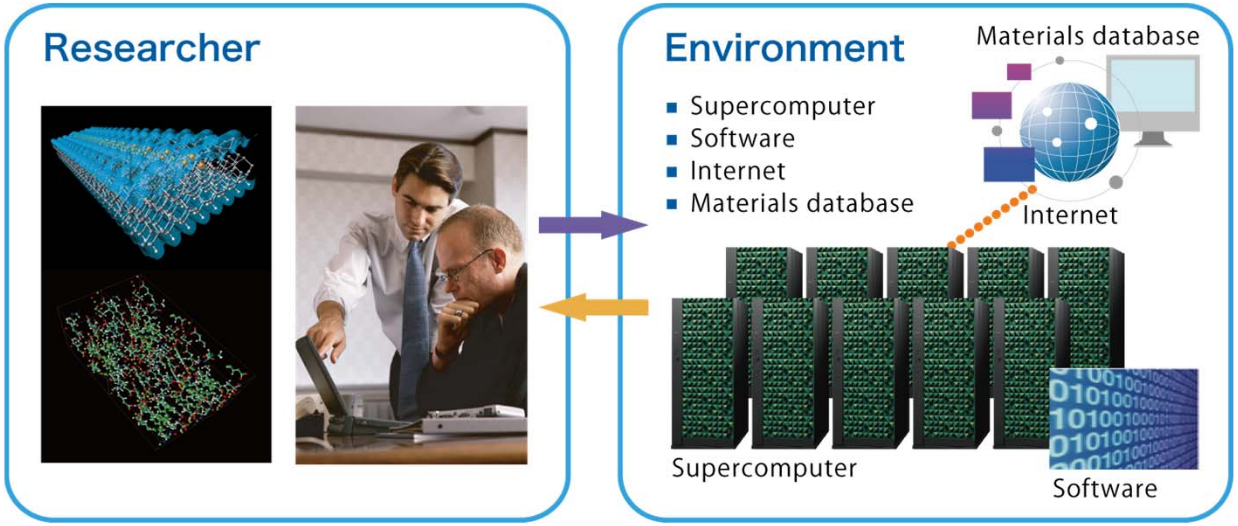


1) *Nature* 499, 2013; 316–319; doi:10.1038/nature12340

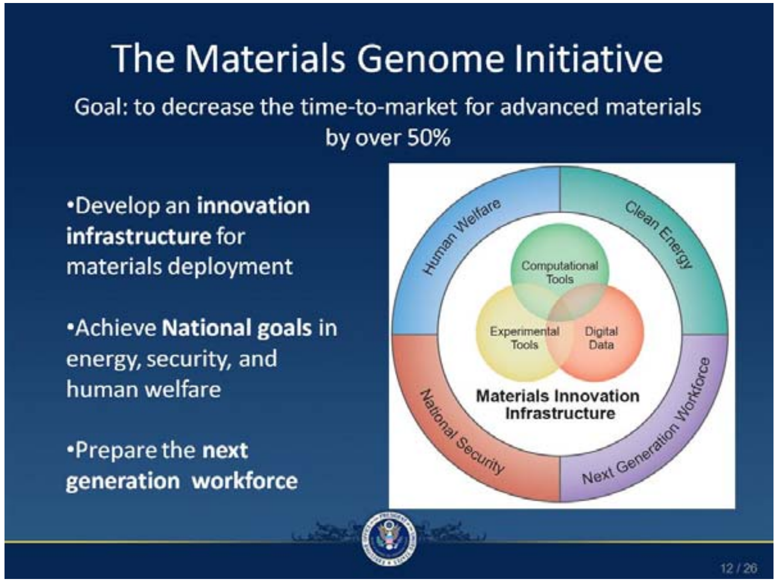
Semiconductors & Electronics: Materials Modeling & Design

- **Computational materials science** is seeing **significant government investment** (e.g., €5 million for NoMaD, $500 million for the MGI,)[1,2]
- **Sophisticated** new **techniques** are in development to **analyze materials data**[3]
- Major applications: **simulating material properties**, building **theoretical models**, **design & screen new materials with new properties**





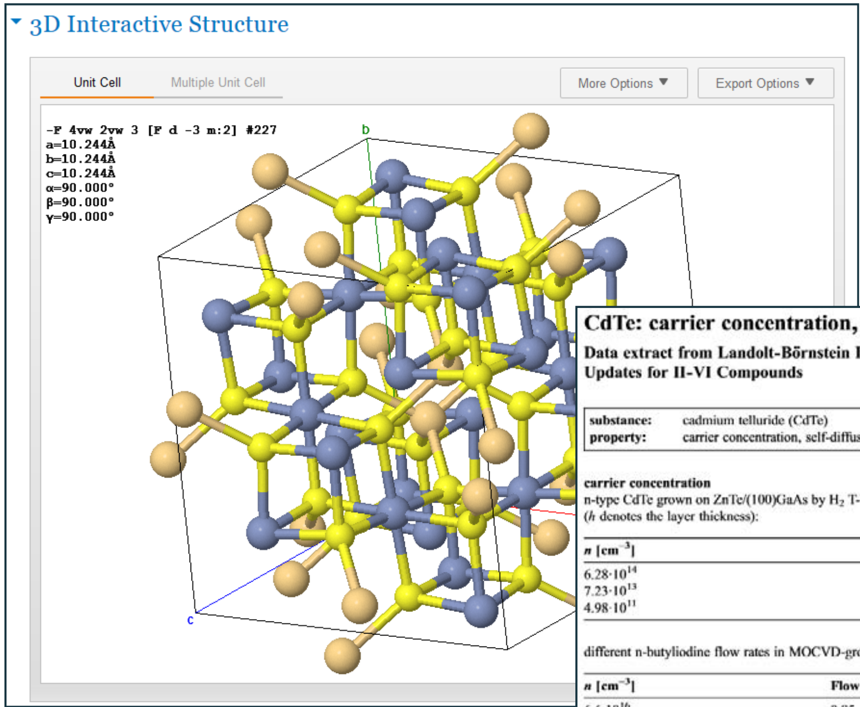
www-lab.imr.tohoku.ac.jp/~ccms/Eng/about/index.php



1) whitehouse.gov/mgi
2) nomad-coe.eu
3) "Can artificial intelligence create the next wonder material?" – *Nature* News Feature. 4 May 2016

Semiconductors & Electronics: Materials Modeling & Design

- Theoretical models require accurate, experimentally validated input data to give meaningful results; calculations also need to be validated by experimental values
- SpringerMaterials can assist materials modeling & design with extensive collections of experimentally verified data for electronic materials applications



CdTe: carrier concentration, self-diffusion

Data extract from Landolt-Börnstein III/44B: Semiconductors – New Data and Updates for II-VI Compounds

substance: cadmium telluride (CdTe)
property: carrier concentration, self-diffusion (transport properties)

carrier concentration
n-type CdTe grown on ZnTe/(100)GaAs by H_2 T-VPE at T = 764 °C as a function of the epilayer thickness (h denotes the layer thickness):

n [cm^{-3}]	h [μm]	Ref.
$6.28 \cdot 10^{14}$	8.76	00L
$7.23 \cdot 10^{13}$	22.1	
$4.98 \cdot 10^{11}$	29.3	

different n-butyliodine flow rates in MOCVD-grown epilayers (T_{growth} = 150 °C):

n [cm^{-3}]	Flow rate [μmol/min]	Ref.
$6.6 \cdot 10^{16}$	0.85	02N
$1.12 \cdot 10^{17}$	1.2	
$1.18 \cdot 10^{18}$	1.41	

chemical self-diffusion coefficient

D [cm^2/s]	T [°C]	Ref.
$2.5(8) \cdot 10^{-7}$	500	02G
$1.7(5) \cdot 10^{-6}$	600	
$>4 \cdot 10^{-6}$	700	

$Ba_2Cu_{2.7}Zn_{0.3}YO_7$ rt charge carrier concentration

General Information

Hermann Mauguin Symbol(s): *Pmmm*
Phase Label(s): $Ba_2Cu_{2.7}Zn_{0.3}YO_7$ rt
Structure Class(es): high-T_c cuprate family
Property Class(es): antiferromagnet AFM, diamagnetic, high-T_c superconductor, intermediate valence, metal, nonmetal, superconductor
Mineral Name(s): –
Pearson Symbol: *oP*14
Space Group: 47
Phase Prototype: $Ba_2Cu_3YO_7$
Compound Class(es): oxide

Property	Temperature	Specimen Details	Remark	ISP ID	Reference
$n_e + n_h = 5.5\ 10^{27}\ m^{-3}$	–	Ba2Cu2.85Zn0.15YO7 prepared using solid state reaction technique		P1105627	80100. Zhao (1989)
$n_e = 5.45\ 10^{27}\ m^{-3}$	–	Ba2Cu2.8Zn0.2YO6.9 sintered at 1203 K for 24 h		P1811429	106741. He (1988)
$n_e = 7.05\ 10^{27}\ m^{-3}$	T = 280 K	Ba2Cu2.85Zn0.15YO7 mixed under ethanol, dried at ~343 K, heated at 1193 K for 50 h with two intermediate grindings, pressed, sintered at 1223 K for 24 h, furnace-cooled no other phases detected by X-ray diffraction	from Hall resistivity measurements dnH/dT = 1.5 1025 m−3 K−1	P1904127	106569. Affronte (1989)

Metals, Alloys, Ceramics: Refractory Metals

- **Refractory metals** and alloys are high melting (>2,000 °C) materials based on Nb, Ta, Mo, W, and Re
- Refractory metals have **extremely high heat and corrosion resistance**
- The high stability of refractory metals makes them **widely used** in numerous **consumer and industrial applications**:

periodictable.com

Chemical reactors (Ta)

mersen.com

Superconductors (Nb)

brainimaging.waisman.wisc.edu/facilities/MRI.html

Tubing (Mo)

tubehollows.com

Rocket Nozzles (W)

Resolution-class submarine

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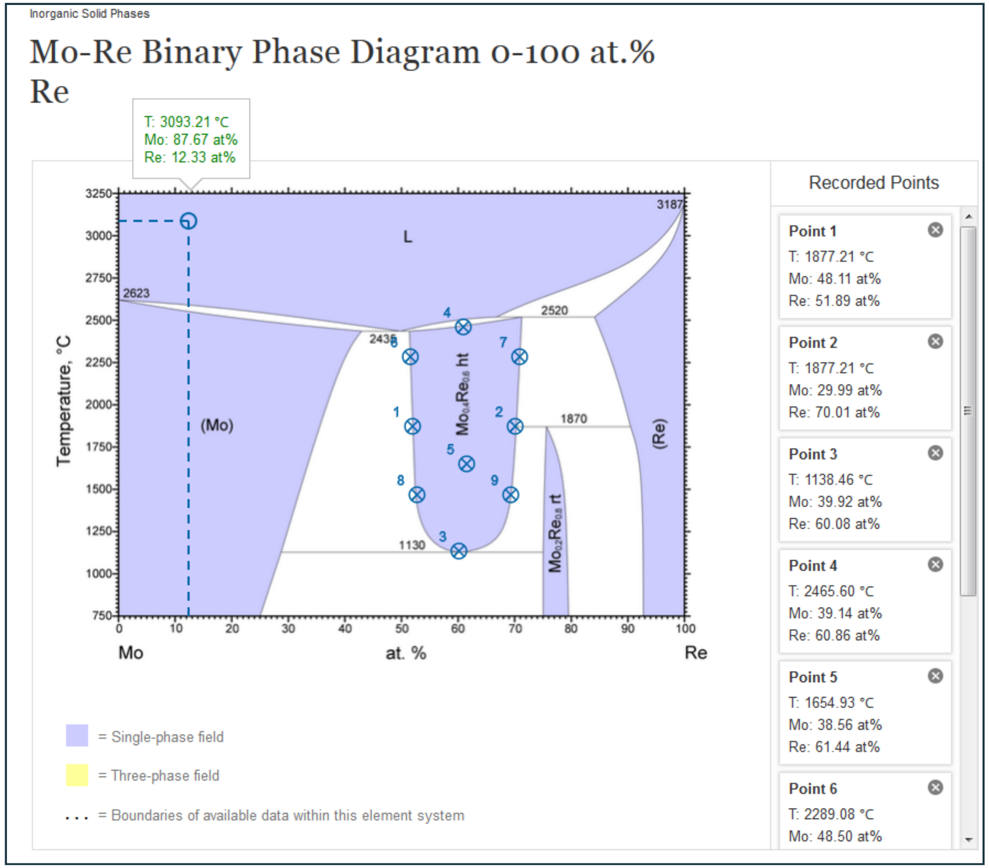
Metals, Alloys, Ceramics: Refractory Metals

- Mo often alloyed with Re to enhance ductility, typically for high temperature applications: thermocouples, furnace parts, welding, etc.
- In the Mo-Re alloy, a brittle phase exists (σ, ~Mo_2Re_3) [1]
- Users can search for the Mo-Re phase diagram to find the conditions where the brittle phase occurs



General Information

Apdic: non-APDIC
Concentration Range: T[600-3250 °C] vs. Re conc.[0-100 at.%]
Investigation Type: experimental, detailed
Temperature: 750...3250 °C (1023...3523 K)

List of Phases

Phase Label	Published Phase Label	Phase Prototype	Pearson Symbol	Hermann Mauguin Symbol	Space Group	Reference	Crystallographic Datasheet
(Re)	Re	Mg	*hP2*	*P6₃/mmc*	194	99574. Savitskii (1969)	SD0528532
$Mo_{0.2}Re_{0.8}$ rt	χ	Mn	*cI58*	*I-43m*	217	47852. Knapton (1958/59)	SD0535180
$Mo_{0.4}Re_{0.6}$ ht	σ	$(Cr_{0.49}Fe_{0.51})$	*tP30*	$P4_2/mnm$	136	4343. Wilson (1963)	SD0451571
(Mo)	Mo	W	*cI2*	*Im-3m*	229	27997. Vavilova (1991)	SD0310446

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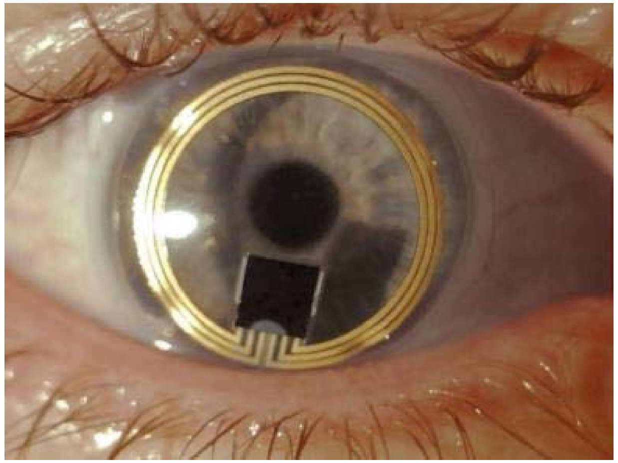
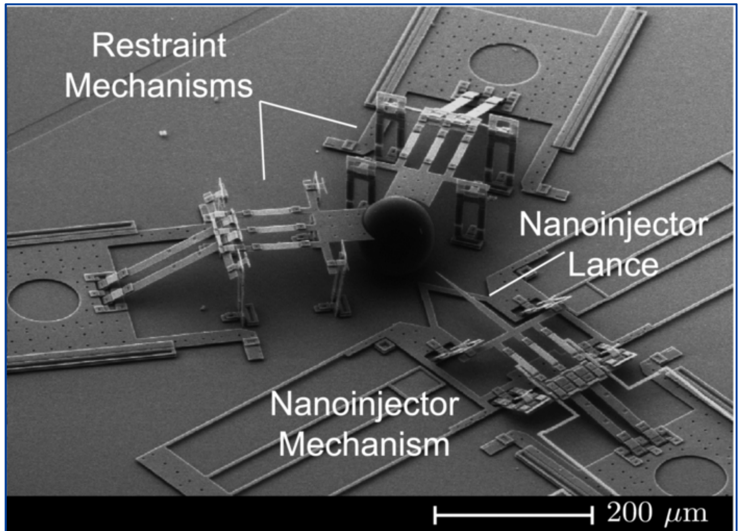
1) *J. Mater. Eng. Perf.* 1994 , 3, 282-291

Metals, Alloys, Ceramics: Microelectromechanical Systems (MEMS)

- **Microelectromechanical Systems (MEMS)** are devices combining electrical and mechanical components on the micro (10^{-6} m) scale
- MEMS are **closely related** to the smaller (10^{-9} m) **nanoscale** materials
- The **fast growing market** of MEMS applications includes **drug delivery**, **inertial sensors**, **chemical detection**, and much more



memsjournal.com/2009/02/applying-mems-technology-to-the-diagnosis-of-glaucoma-.html



(a) SEM of a nanoinjector

scitation.aip.org/content/aip/journal/rsi/85/5/10.1063/1.4872077

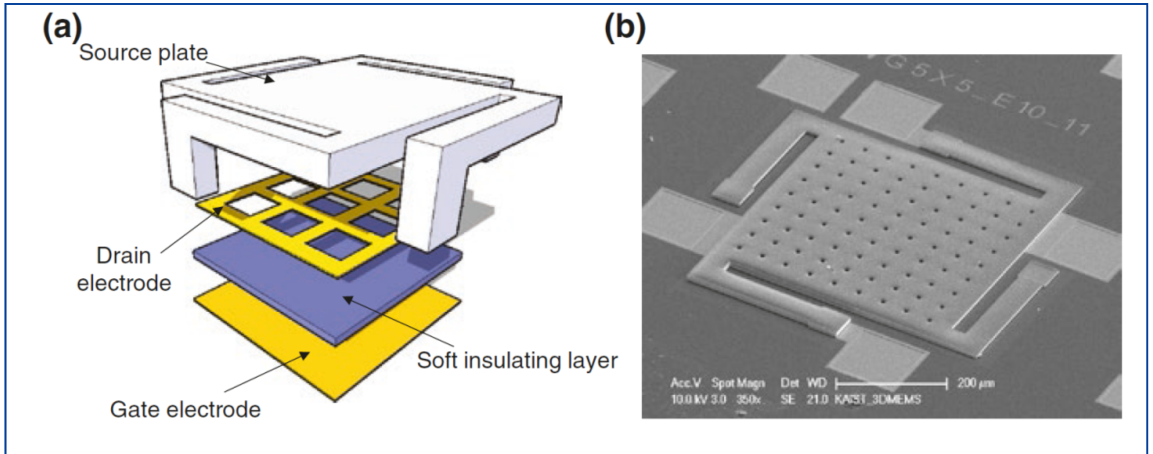
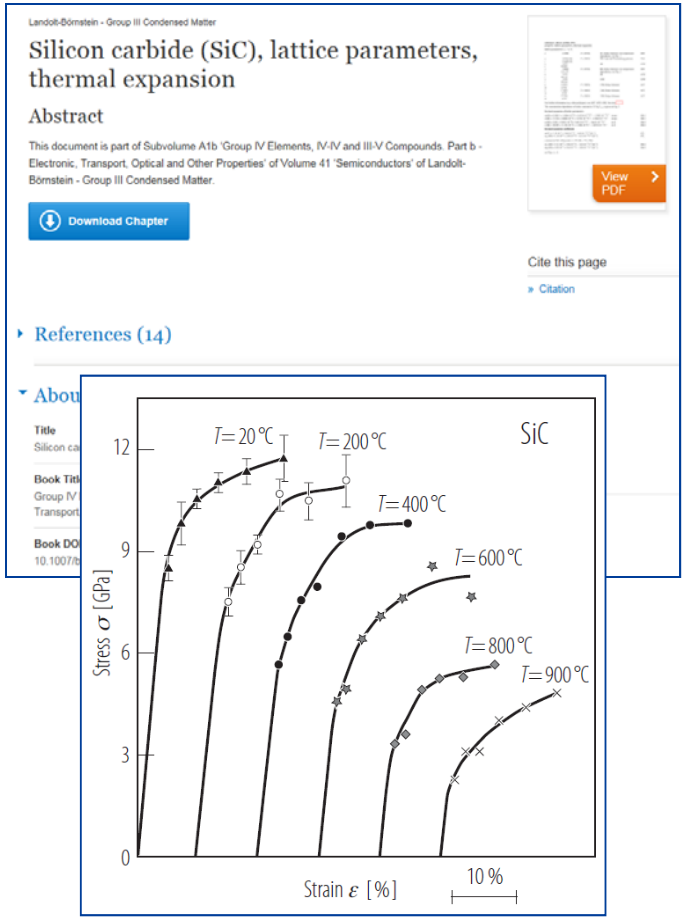


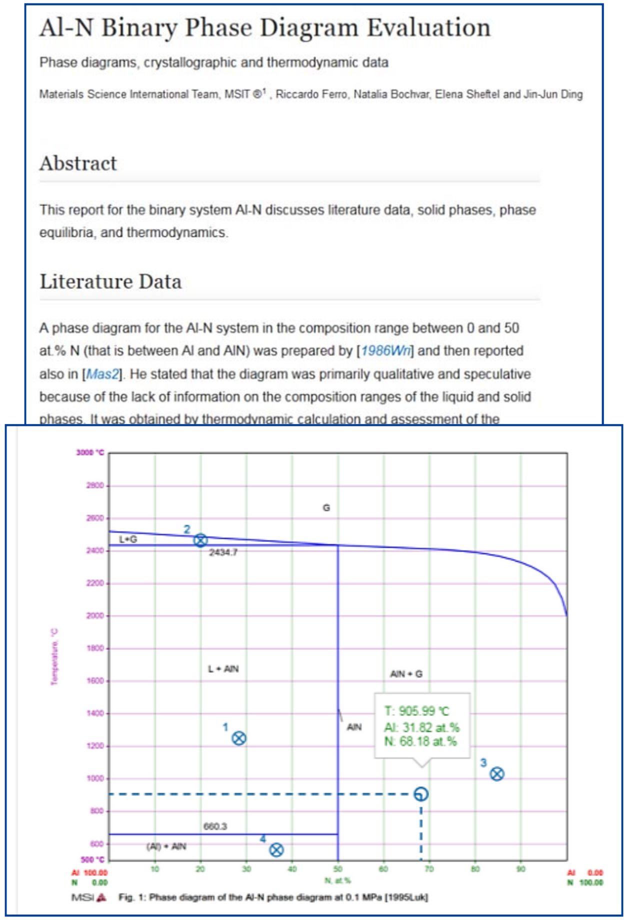
Fig. 11 **a** Schematic illustration and **b** SEM image of the stacked electrode MEMS switch with a soft insulating layer [33]

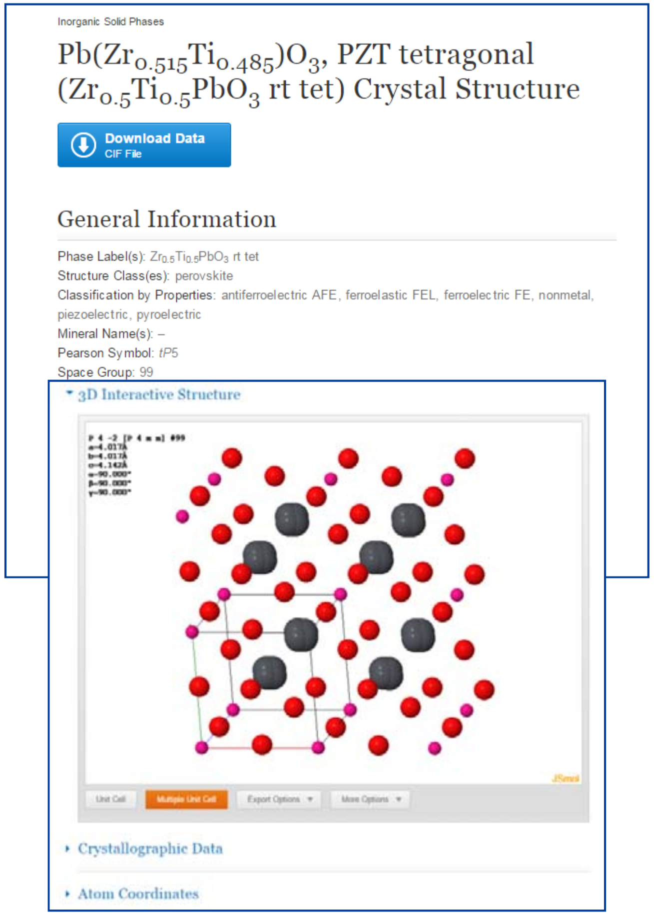
Kyung Chong-Min, ed. Nano Devices and Circuit Techniques for Low-Energy Applications and Energy Harvesting, Springer 2016.

Metals, Alloys, Ceramics: Microelectromechanical Systems (MEMS)

- MEMS devices are traditionally silicon-based but increasingly use a variety of ceramic-based materials
- SpringerMaterials contains extensive data on the structural, mechanical, thermal, electronic, and optical properties of the ceramics used in MEMS research:



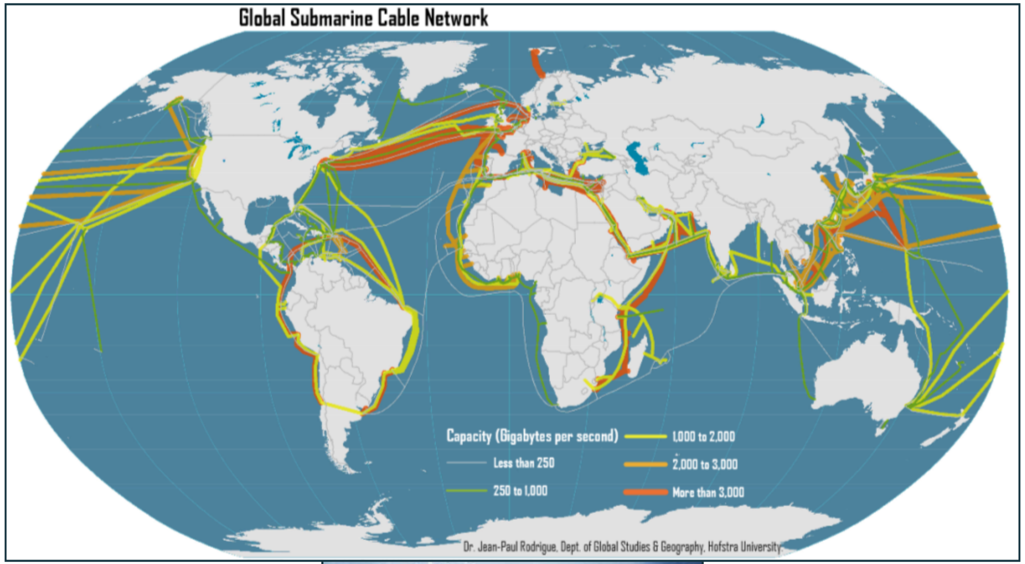




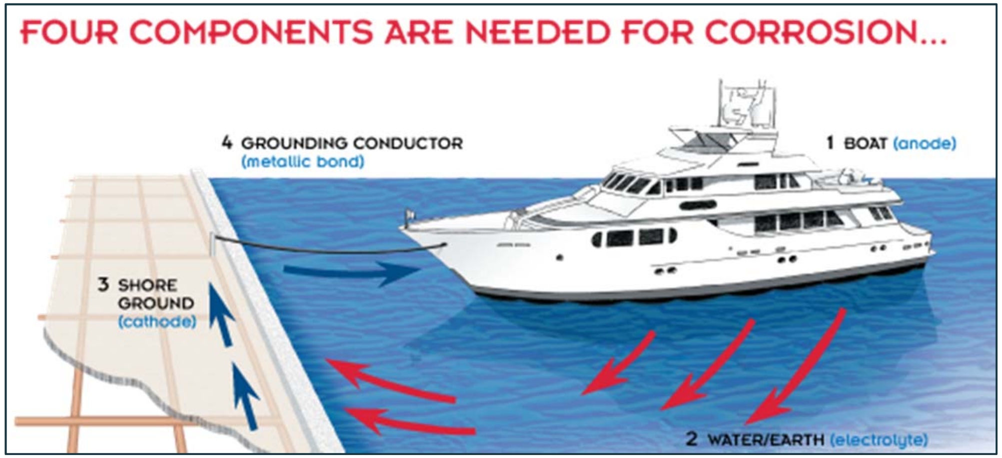
Metals, Alloys, Ceramics: Marine Corrosion

- **Marine corrosion** occurs when materials are in contact with seawater
- Marine corrosion affects major industries globally; **shipping & transportation, oil & gas, and IT**
- Yearly **cost**[1] of marine corrosion: $50–80 billion

jotun.com/aa/en/b2b/paintsandcoatings/offshore-installations/



Greg's Cable Map



deimarine.com/galvanic-corrosion

1) Corrosion in the Maritime Industry: NACE International

Metals, Alloys, Ceramics: Marine Corrosion

- SpringerMaterials has an extensive Corrosion Database with detailed exposure data for hundreds of metals & alloys in seawater
- Data is easily sortable, allowing quick determination of most/least resistant materials

Corrosion Search

Find out a corrosion rate and its relevant details by entering a material and/or environment into the search box below.

environment: Seawater ×

Enter material and/or environment

367 results — 1 of 37

Material ▲	Environment	Rating	Show all details
0.3Cu steel	Seawater	Localized	More details
0.3Cu steel	Seawater	B (Good) 0.15 mm/year	More details
0.3Cu steel	Seawater	A (Resistant) 0.089 mm/year	More details
0.3Cu steel	Seawater	A (Resistant) 0.079 mm/year	More details
0.3Cu steel	Seawater	Localized	More details
0.3Cu steel	Seawater	Localized	More details
1.2Mn-0.75Ni-0.45Cu steel	Seawater	A (Resistant) 0.11 mm/year	More details
1.2Mn-0.75Ni-0.45Cu steel	Seawater	A (Resistant) 0.097 mm/year	More details
1.2Mn-0.75Ni-0.45Cu steel	Seawater	A (Resistant) 0.08 mm/year	More details

Corrosion Search

Find out a corrosion rate and its relevant details by entering a material and/or environment into the search box below.

environment: Seawater × material: 0.3Cu steel × material: 301 stainless steel ×

Enter material and/or environment

8 results — 1 of 1

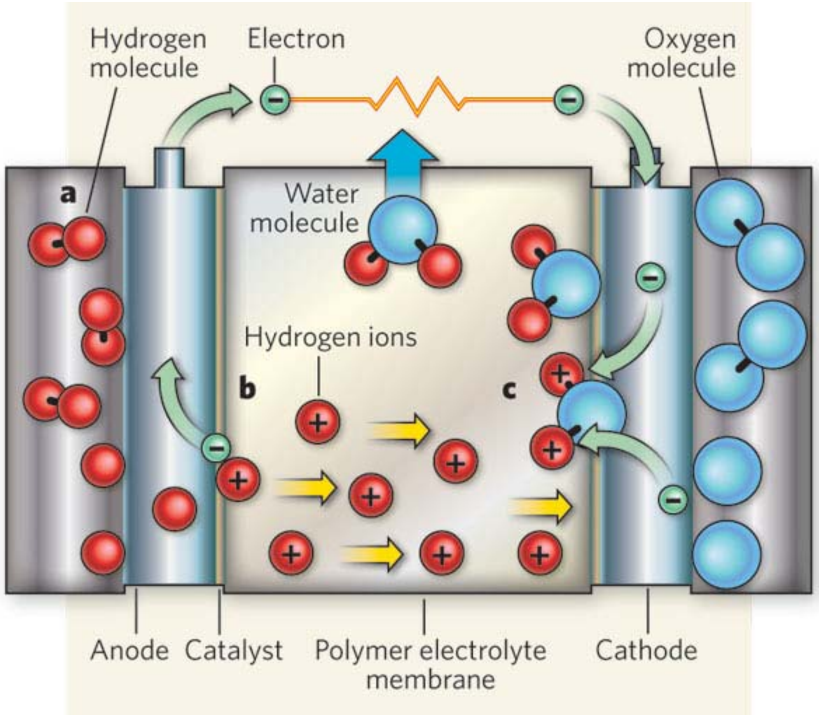
Material	Environment	Rating ▲	Show all details
301 stainless steel	Seawater	A (Resistant) ≤ 0.125 mm/year	
Condition:	**Temperature:** 20.0 °C	**Duration:** **Localised attack:** pitting	
UNS No: S30100	**Reference:** Chemical Resistance of REMANIT Stainless Steels, Thyssen Edelstahlwerke AG, March 1989		Less details
0.3Cu steel	Seawater	A (Resistant) 0.079 mm/year	More details
0.3Cu steel	Seawater	A (Resistant) 0.089 mm/year	More details
0.3Cu steel	Seawater	B (Good) 0.15 mm/year	More details
301 stainless steel	Seawater	C (Questionable) 0.5 - 1.25 mm/year	More details

Chemical Processing & Energy Applications: Hydrogen Purification

- **Hydrogen gas** is an essential component in **dozens** of industrial processes (ammonia synthesis, oil refining, desulfurization, methanol production, etc.)
- Hydrogen is also a key component in the growing **fuel cell market** (valued at ~$2.2 billion in 2014)[1]
- Applications for hydrogen-based fuel cells include **vehicle and device batteries**

Kticorp.com/SteamReformers.htm

Hydrogen-powered 2016 Toyota Mirai

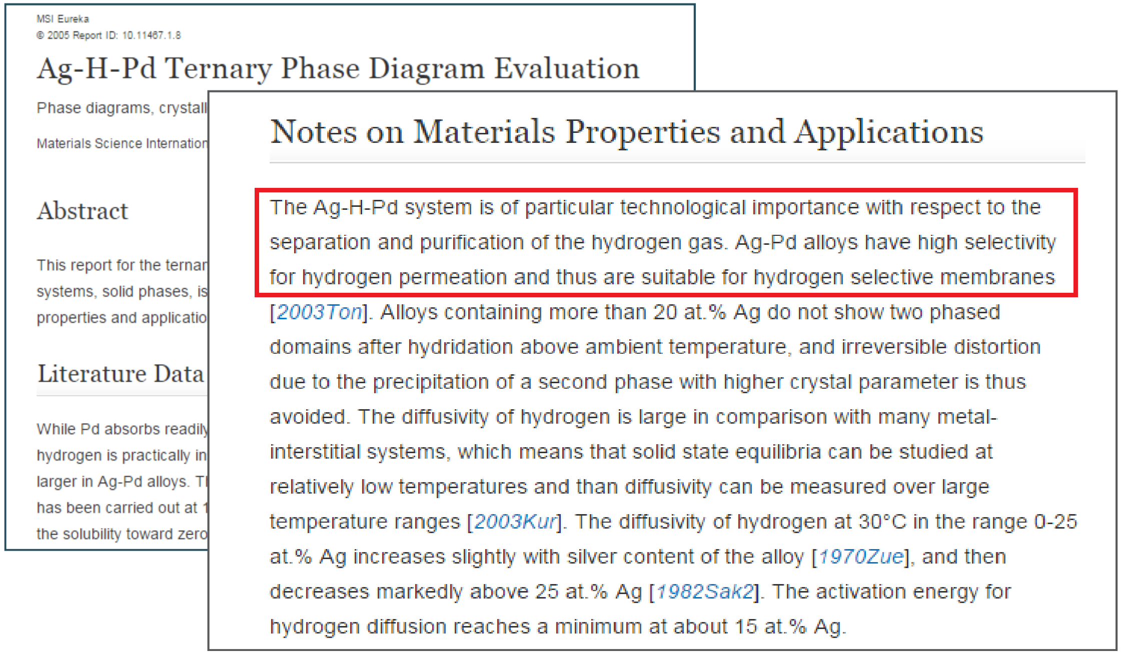


Nature 460, 2009; 809–311; doi:10.1038/460809a

1) "Fuel Cell Technologies Market Report 2014", US Dept. of Energy, Oct. 2015.

Chemical Processing & Energy Applications: Hydrogen Purification

- Byproducts are common in many H_2 production processes (e.g., steam reforming)
- Researchers can use SpringerMaterials to search for the most appropriate materials to purify H_2 and optimize production for the desired scale and application:



MSI Eureka
© 2005 Report ID: 10.11467.1.8

Ag-H-Pd Ternary Phase Diagram Evaluation

Phase diagrams, crystall

Materials Science Internation

Abstract

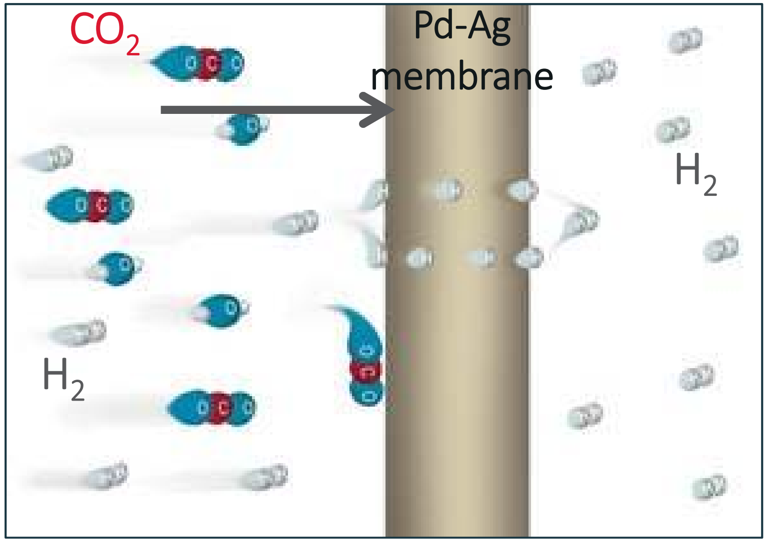
This report for the ternar
systems, solid phases, is
properties and applicatio

Literature Data

While Pd absorbs readily
hydrogen is practically in
larger in Ag-Pd alloys. T
has been carried out at 1
the solubility toward zero

Notes on Materials Properties and Applications

The Ag-H-Pd system is of particular technological importance with respect to the separation and purification of the hydrogen gas. Ag-Pd alloys have high selectivity for hydrogen permeation and thus are suitable for hydrogen selective membranes [2003Ton]. Alloys containing more than 20 at.% Ag do not show two phased domains after hydridation above ambient temperature, and irreversible distortion due to the precipitation of a second phase with higher crystal parameter is thus avoided. The diffusivity of hydrogen is large in comparison with many metal-interstitial systems, which means that solid state equilibria can be studied at relatively low temperatures and than diffusivity can be measured over large temperature ranges [2003Kur]. The diffusivity of hydrogen at 30°C in the range 0-25 at.% Ag increases slightly with silver content of the alloy [1970Zue], and then decreases markedly above 25 at.% Ag [1982Sak2]. The activation energy for hydrogen diffusion reaches a minimum at about 15 at.% Ag.



For $Pd_{0.75}Ag_{0.25}$ alloy, the permeability of H_2 is given by the following design equation:

$$R_{H2} = 46 \cdot 10^{-9} \left(\frac{A}{H}\right) \left(\rho_H^{\frac{1}{2}} - \rho_L^{\frac{1}{2}}\right) e^{\left(-\frac{794}{T}\right)} \, mol \cdot min^{-1}$$

Where A = membrane area (cm^2), H = membrane thickness (cm), ρ_H = driving pressure, (Pa) ρ_L = back pressure (Pa), T = temperature (K)

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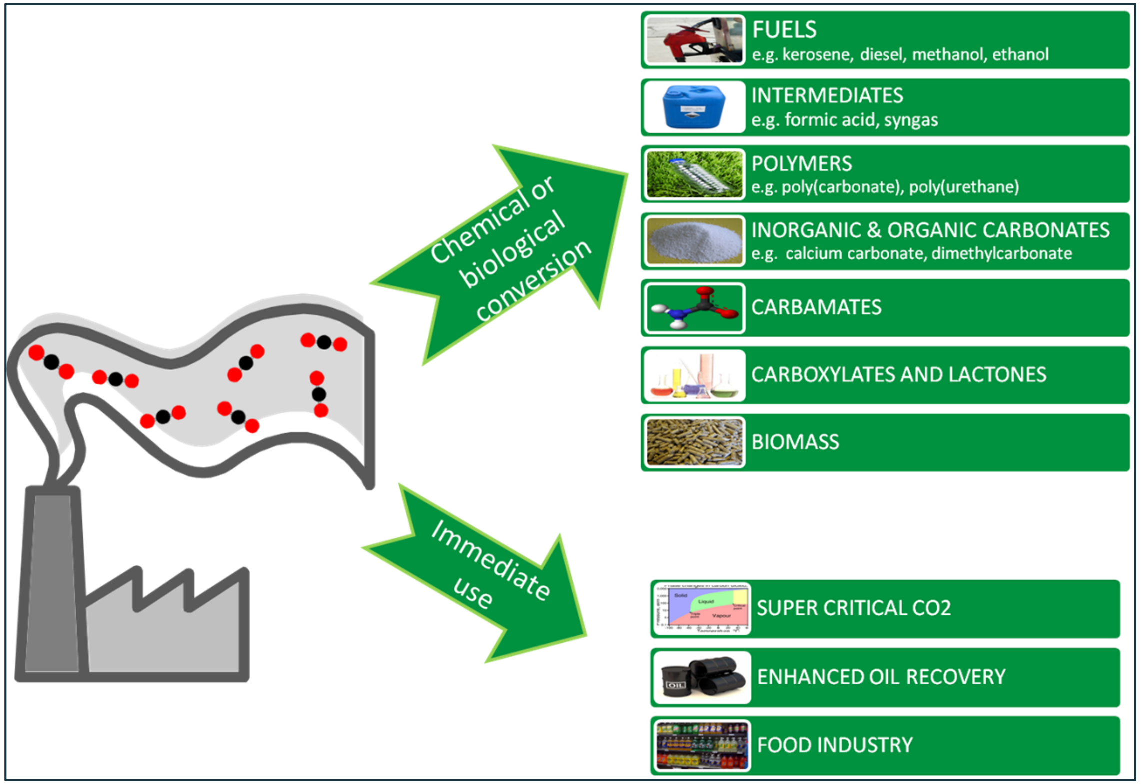
Chemical Processing & Energy Applications: CO_2 Capture & Utilization

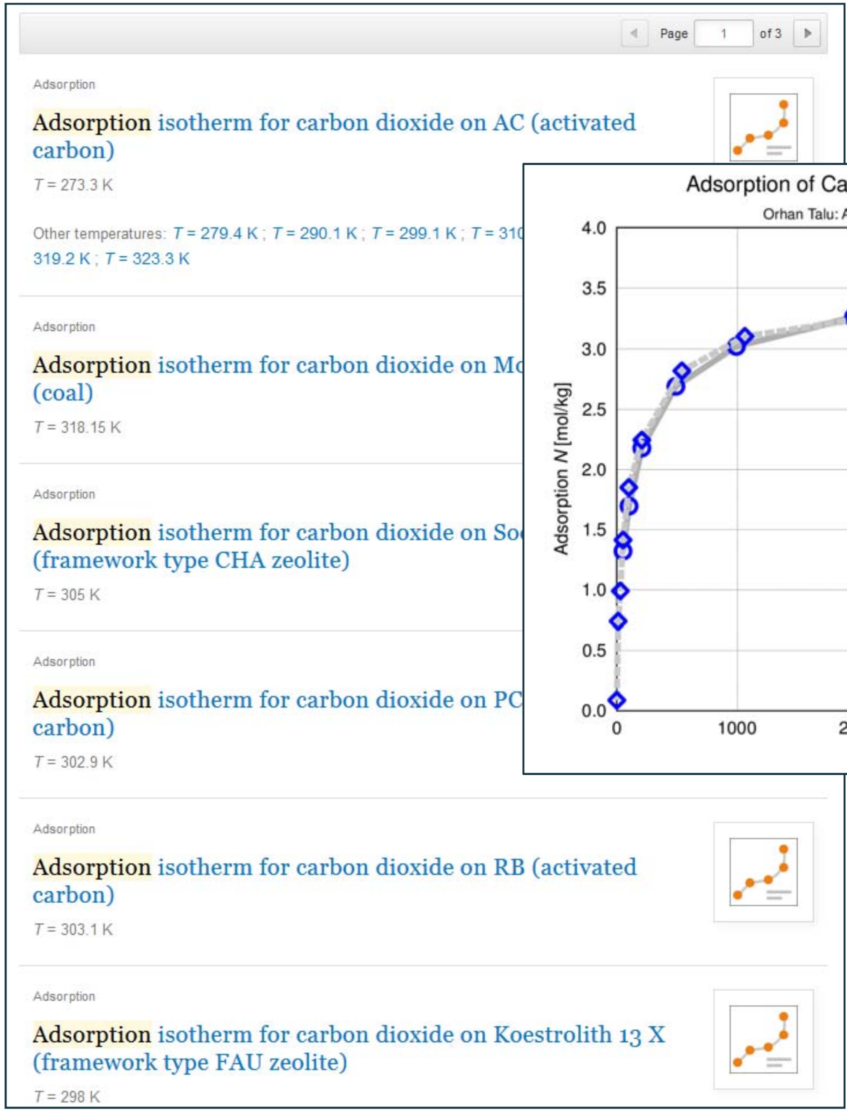
- Managing **carbon dioxide emissions** is a prominent issue[1] in **international politics**
- The **capture, storage, and reuse** of **carbon dioxide** is being actively investigated[2,3]
- Captured **carbon dioxide** can be used in the **production** of **many important materials** (polyurethanes, benzene, diesel, methanol, etc.)



1) unfccc.int/paris_agreement/items/9485.php
2) chemanager-online.com/en/topics/chemicals-distribution/co2-feedstock-fuels-chemistry-and-polymers3
3) pbs.org/wgbh/nova/next/tech/beccs

Chemical Processing & Energy Applications: CO_2 Capture & Utilization

- SpringerMaterials has extensive analytical & spectroscopic data on the adsorption/desorption of CO_2 on numerous materials and in many conditions



Page 1 of 3

Adsorption

Adsorption isotherm for carbon dioxide on AC (activated carbon)

T = 273.3 K

Other temperatures: T = 279.4 K ; T = 290.1 K ; T = 299.1 K ; T = 31… 319.2 K ; T = 323.3 K

Adsorption

Adsorption isotherm for carbon dioxide on M… (coal)

T = 318.15 K

Adsorption

Adsorption isotherm for carbon dioxide on So… (framework type CHA zeolite)

T = 305 K

Adsorption

Adsorption isotherm for carbon dioxide on PC… carbon)

T = 302.9 K

Adsorption

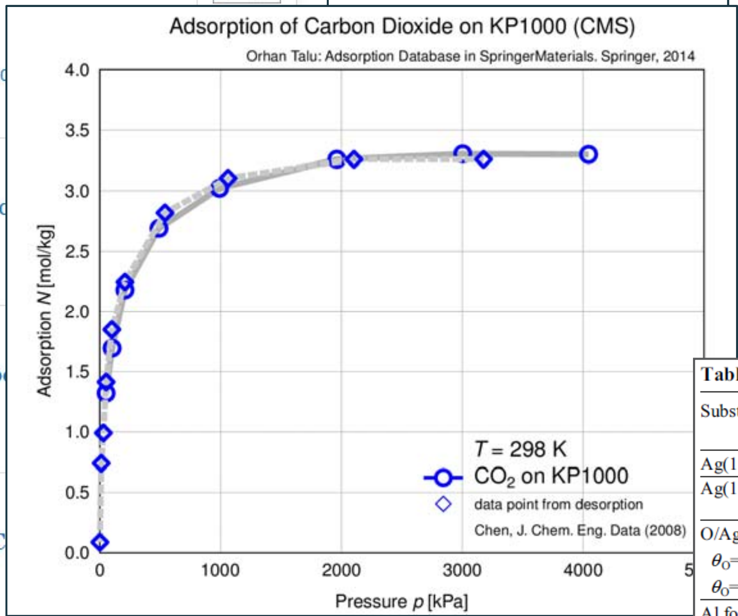
Adsorption isotherm for carbon dioxide on RB (activated carbon)

T = 303.1 K

Adsorption

Adsorption isotherm for carbon dioxide on Koestrolith 13 X (framework type FAU zeolite)

T = 298 K



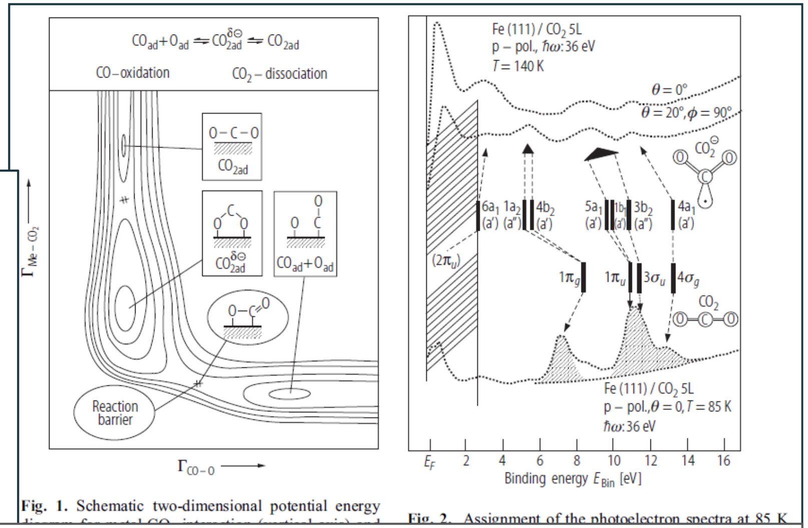


Fig. 1. Schematic two-dimensional potential energy

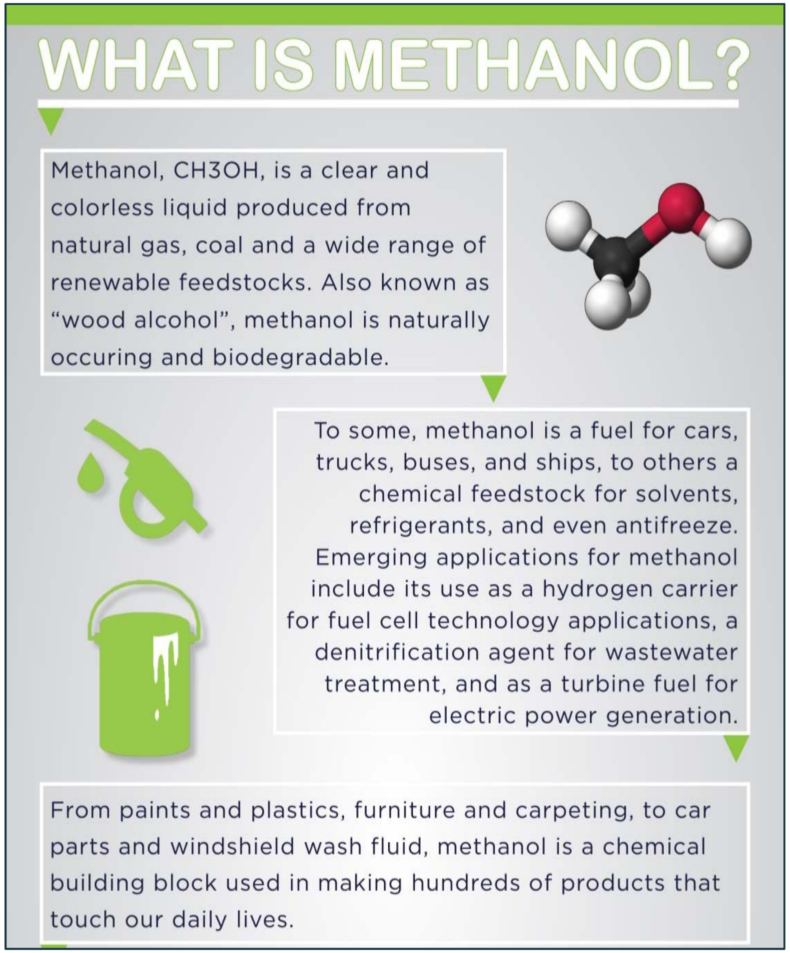
Fig. 2. Assignment of the photoelectron spectra at 85 K

Table 1. Thermodynamics of CO_2 adsorption

Substrate	T_s [K]	Chemi-sorption	Coverage	T_{des} [K]	E_d [kJ/mol]	Technique	Ref.
Ag(111)	40	No				TPD	91Soll, 87Sak
Ag(110)	300	No	0.25			TPD	83Bac
	100	No				TPD	82Stu
O/Ag(110)							
θ_O= 0.1	100	Yes		480	84-102	TPD	91Soll, 82Stu
θ_O= 0.25	100	Yes		420	113	TPD	83Bac
Al foil	80	Yes		<295		XPS	87Car
Al(100)	100	No				TPD	91Soll
Na/Al(100)	100	Yes		285		TPD	91Soll
Bi(0001)	80	No				XPS, HREELS	91Bro
Cu film	90	Yes (weak)		<200		XPS	98Poh
Cu(110)	80	No				TPD	89Rod
	130	No				TPD	96Kra
Cu(100)	100	No				XPS, HREELS	91Bro
Cs/Cu(110)							
θ_{Cs}= 1	80	Yes	0.25	500-600		TPD	94Car, 01God
	80	Yes	0.25	370, 500		TPD	89Rod
K/Cu(110)							
θ_K= 0.5	100	Yes		<175		HREELS	95Ons
θ_K= 0.75	130	Yes	Satn.	<160		UPS, XPS	96Kra

Chemical Processing & Energy Applications: Methanol Mixtures

- **Methanol** is a critically important raw material[1] for chemical production and fuel/energy applications
- In 2015, **70 million metric tons** of methanol was produced[2] for a market worth **$55 billion**
- **Materials** made **directly or indirectly from methanol** are **ubiquitous** in everyday life[1]

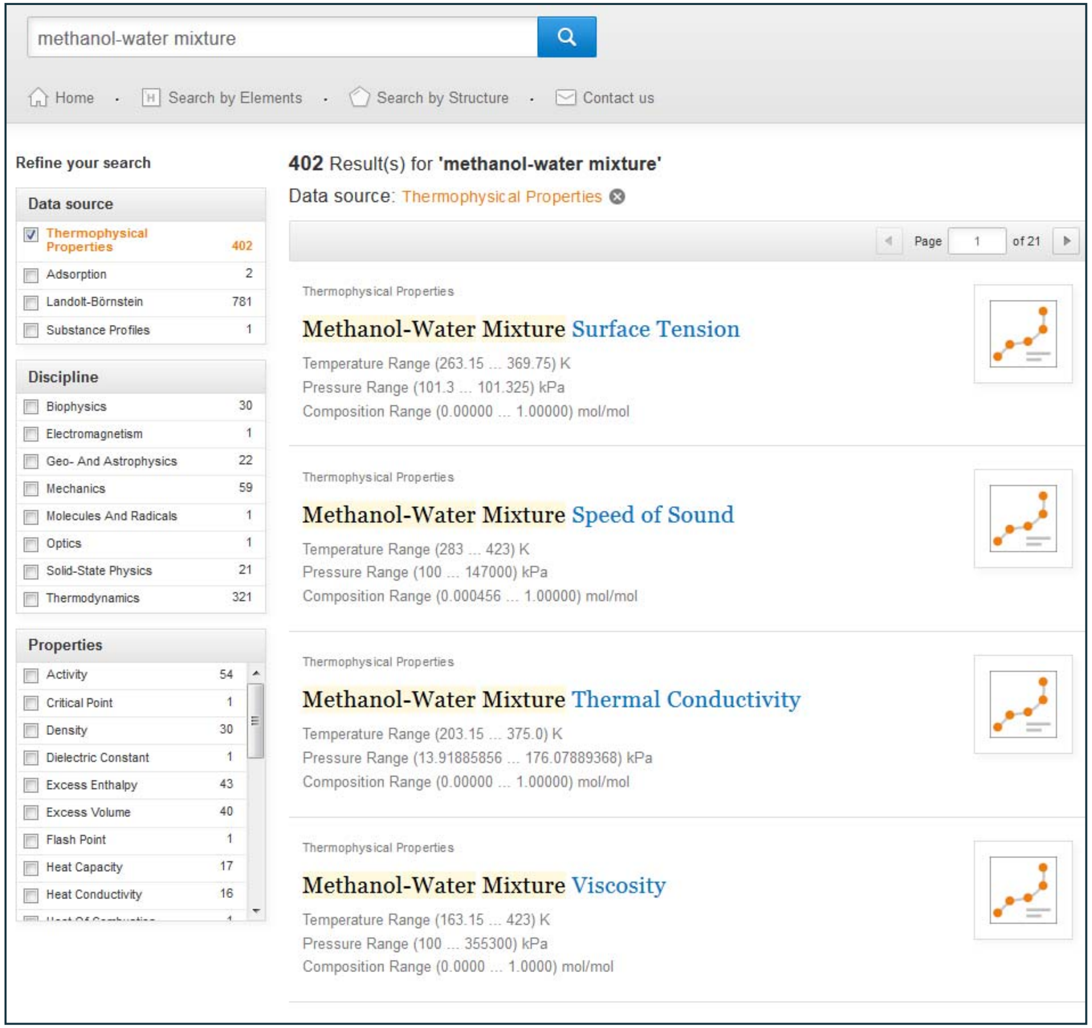


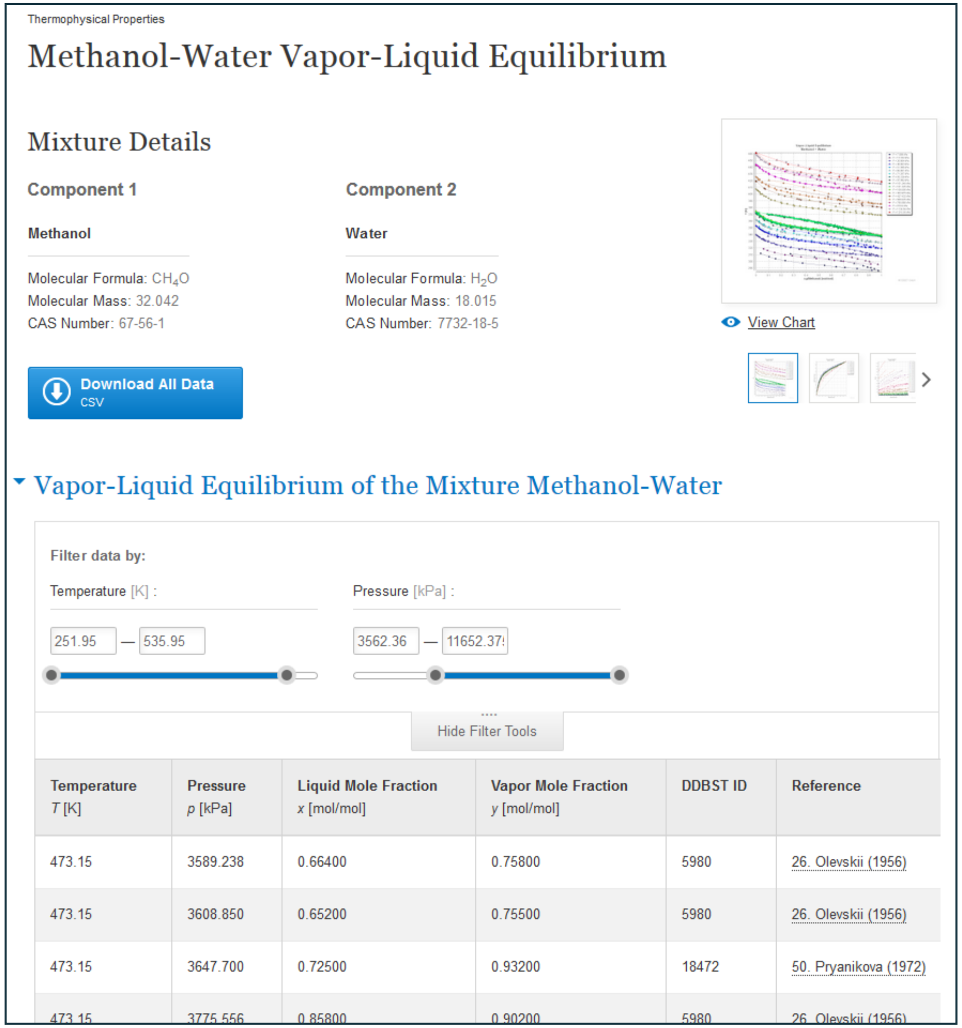
SPRINGER NATURE

1) methanol.org/the-methanol-industry
2) nptel.ac.in/courses/103103029/module3/lec13/3.html

Chemical Processing & Energy Applications: Methanol Mixtures

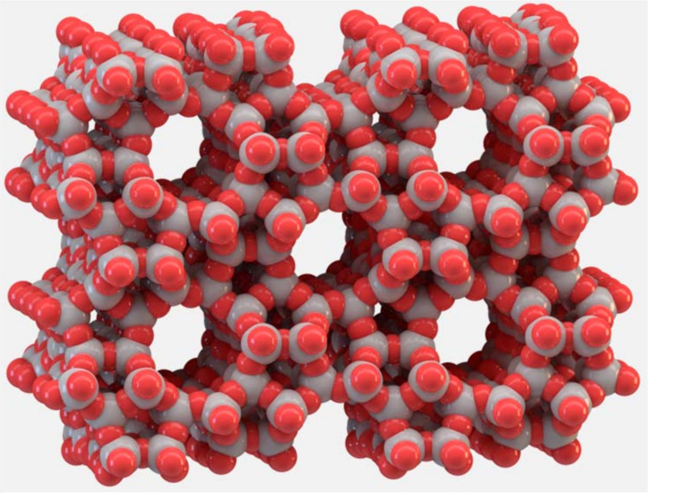
- Methanol is very often produced and used as a water mixture in many processes
- SpringerMaterials supplies numerous thermophysical properties of methanol-water mixtures (e.g., heat capacities, densities, activity coefficients, thermal conductivities):



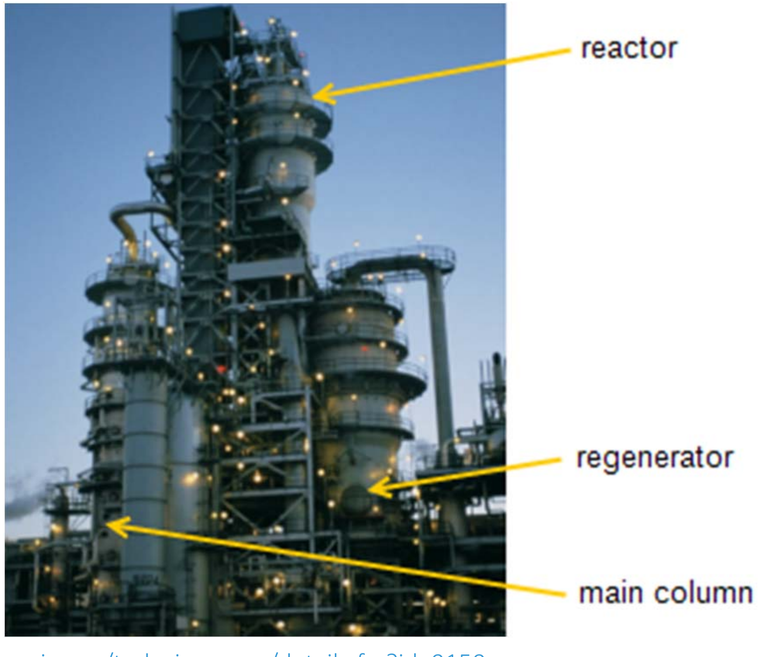


Chemical Processing & Energy Applications: Zeolite Catalysis

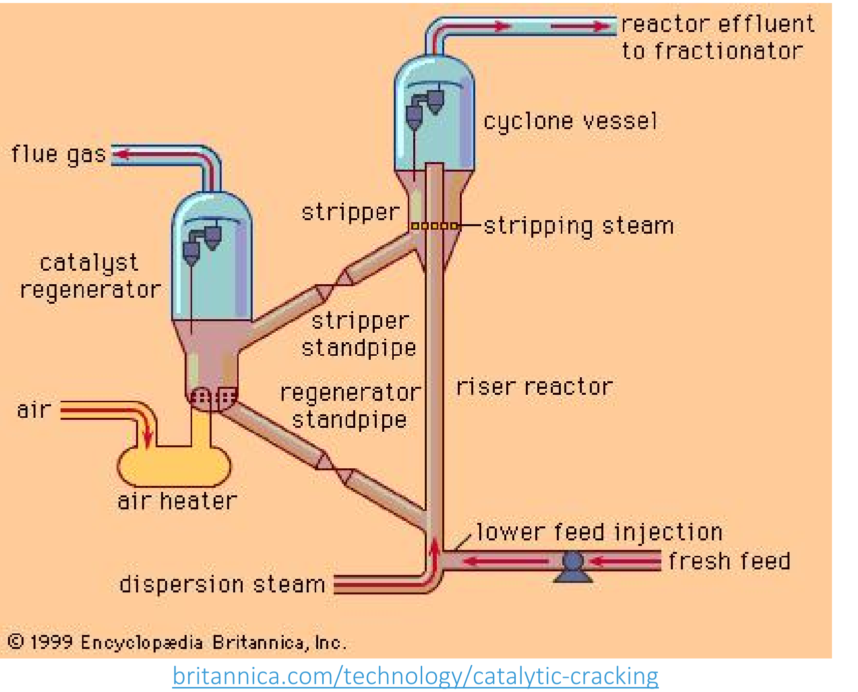
- **Zeolites** are aluminosilicates with highly porous nanostructures
- The **high stability** and **high surface area** of zeolites makes them useful for many applications (e.g., absorbents, ion exchange, gas separation)
- Zeolites are especially important as **catalysts** in **numerous industrial chemical processes** (fluid catalytic cracking, alkylation, oxidation, etc.)



Zeolite ZSM-5 Structure



eia.gov/todayinenergy/detail.cfm?id=9150



britannica.com/technology/catalytic-cracking

Chemical Processing & Energy Applications: Zeolite Catalysis

- Detailed knowledge of zeolite composition and structure is critical for selecting a catalyst with the appropriate selectivity and stability
- SpringerMaterials contains extensive data on the structure and properties of thousands of natural and synthetic zeolites:

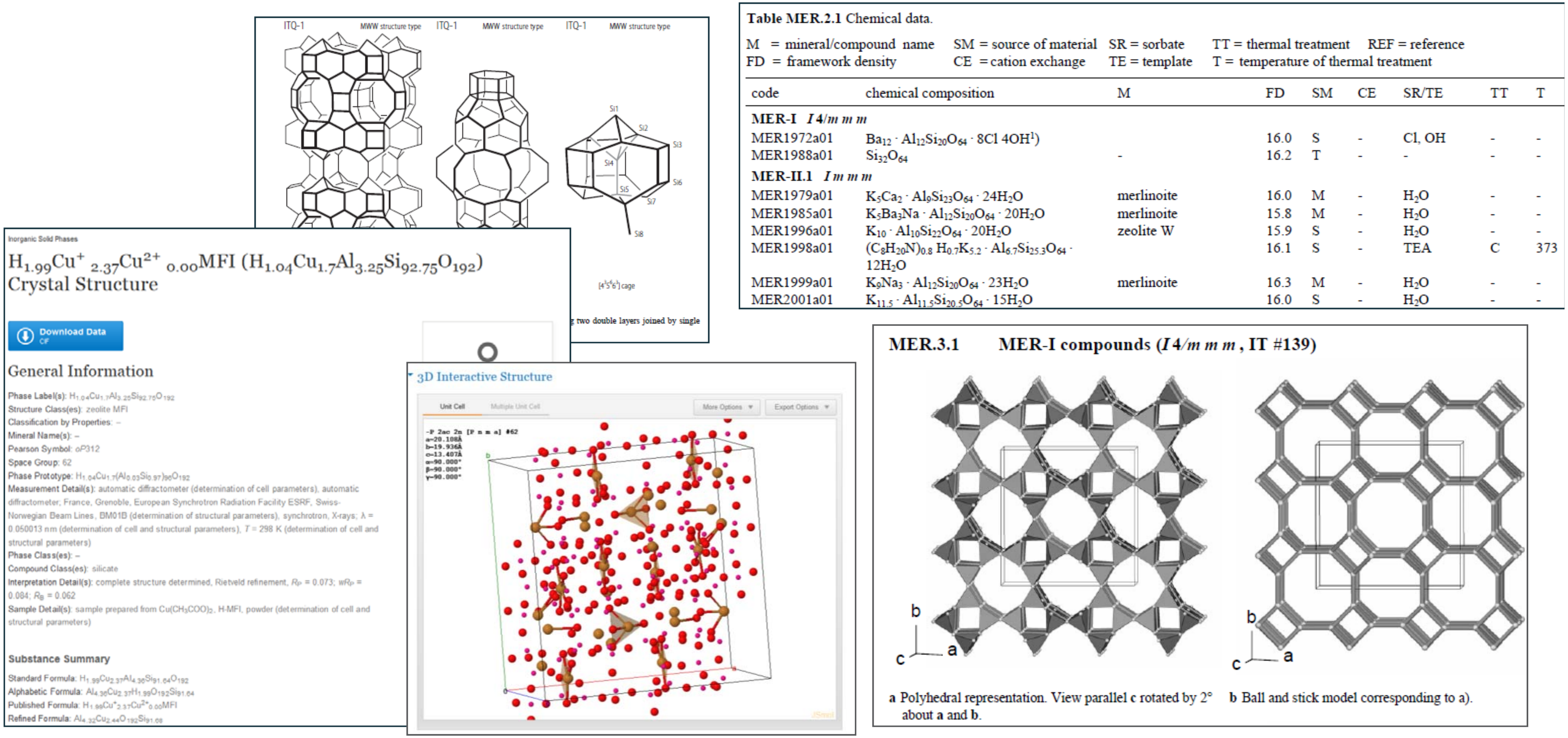


Table MER.2.1 Chemical data.

M = mineral/compound name; SM = source of material; SR = sorbate; TT = thermal treatment; REF = reference
FD = framework density; CE = cation exchange; TE = template; T = temperature of thermal treatment

code	chemical composition	M	FD	SM	CE	SR/TE	TT	T
MER-I *I* 4/*m m m*								
MER1972a01	$Ba_{12} \cdot Al_{12}Si_{20}O_{64} \cdot 8Cl\ 4OH$ [1])		16.0	S	-	Cl, OH	-	-
MER1988a01	$Si_{32}O_{64}$	-	16.2	T	-	-	-	-
MER-II.1 *I m m m*								
MER1979a01	$K_5Ca_2 \cdot Al_9Si_{23}O_{64} \cdot 24H_2O$	merlinoite	16.0	M	-	H_2O	-	-
MER1985a01	$K_5Ba_3Na \cdot Al_{12}Si_{20}O_{64} \cdot 20H_2O$	merlinoite	15.8	M	-	H_2O	-	-
MER1996a01	$K_{10} \cdot Al_{10}Si_{22}O_{64} \cdot 20H_2O$	zeolite W	15.9	S	-	H_2O	-	-
MER1998a01	$(C_8H_{20}N)_{0.8}\ H_{0.7}K_{5.2} \cdot Al_{6.7}Si_{25.3}O_{64} \cdot 12H_2O$		16.1	S	-	TEA	C	373
MER1999a01	$K_9Na_3 \cdot Al_{12}Si_{20}O_{64} \cdot 23H_2O$	merlinoite	16.3	M	-	H_2O	-	-
MER2001a01	$K_{11.5} \cdot Al_{11.5}Si_{20.5}O_{64} \cdot 15H_2O$		16.0	S	-	H_2O	-	-