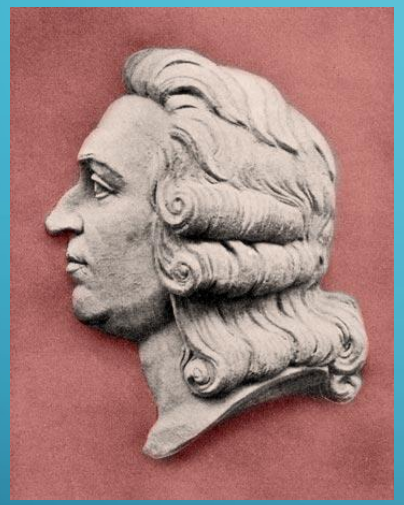
ХИМИЯ ФУНКЦИОНАЛЬНЫХ МАТЕРИАЛОВ

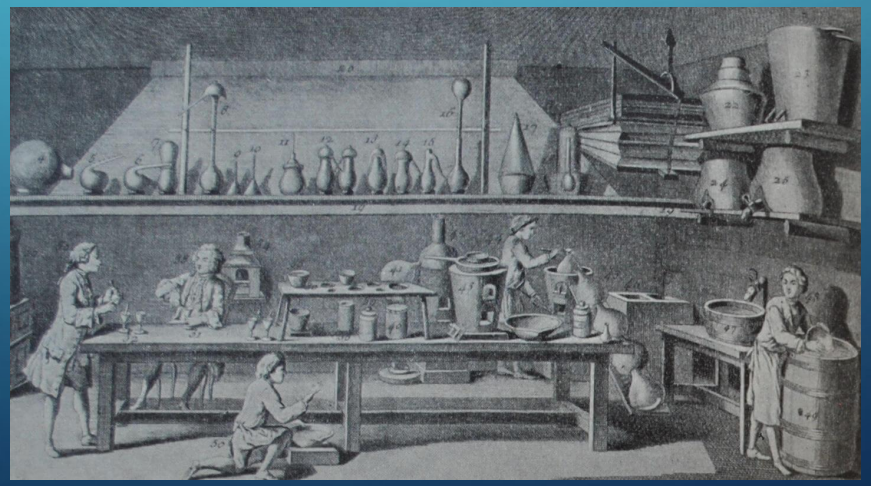
АДСОРБЦИОННЫЕ МАТЕРИАЛЫ. ЦЕОЛИТЫ

ЧТО ЭТО?

1758

Алекс Фредерик Кронштедт



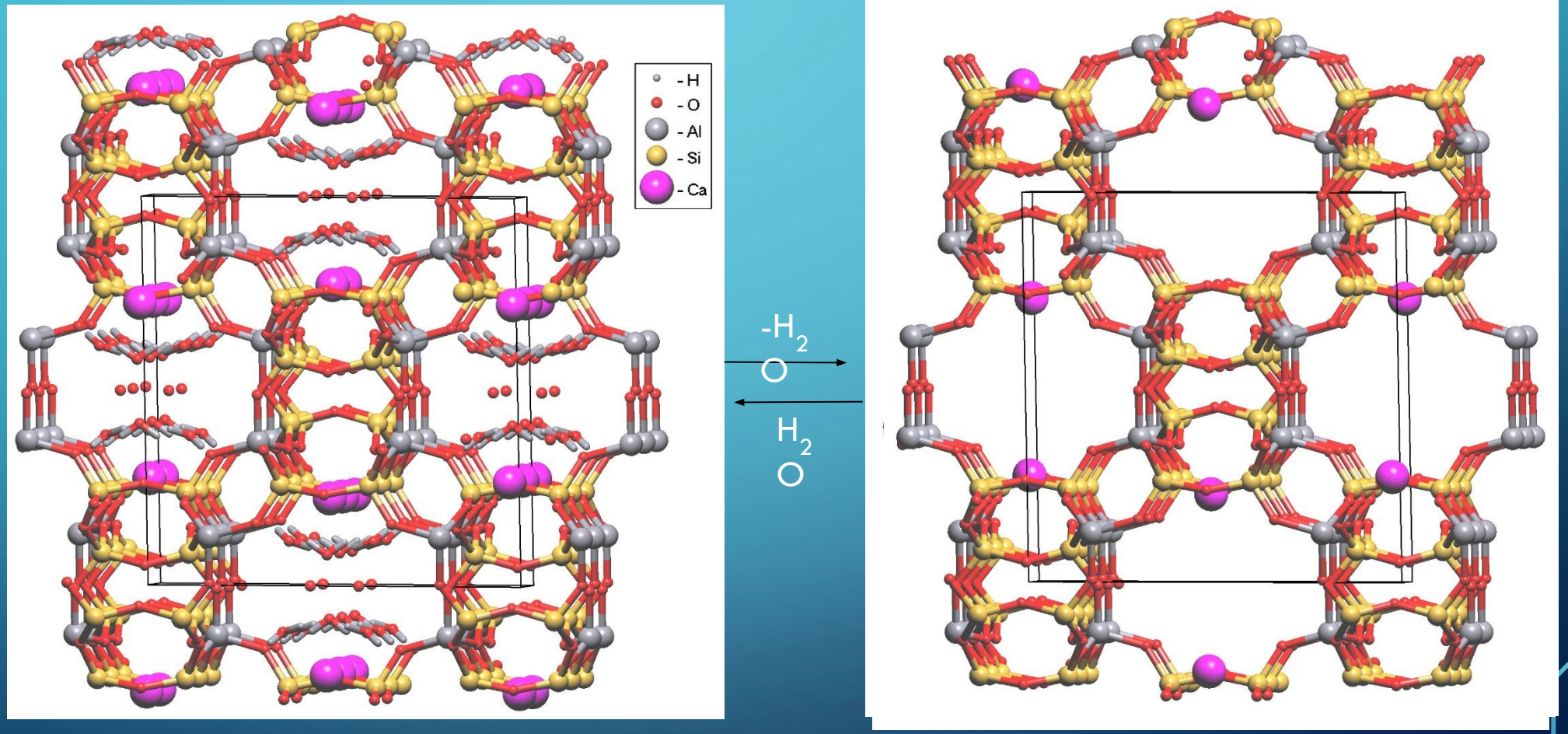


Zein - кипеть

литос- камень

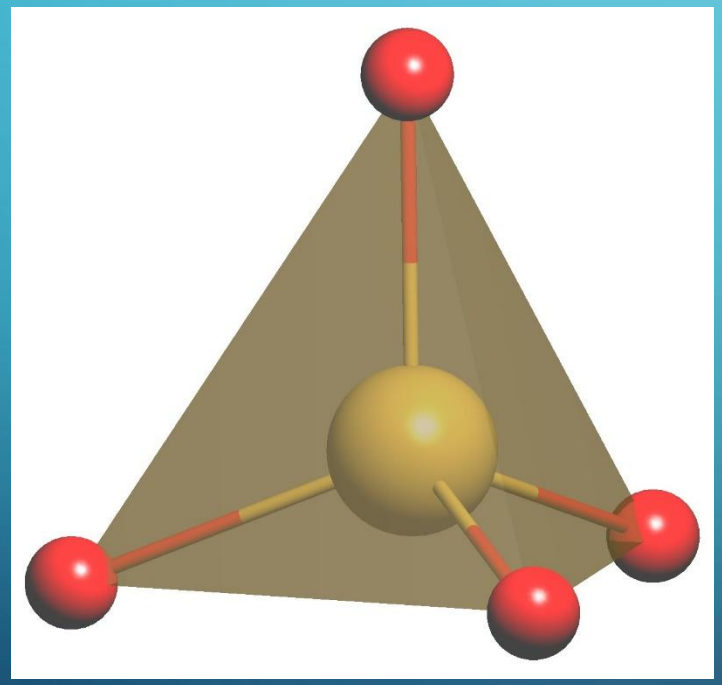
Стильбит

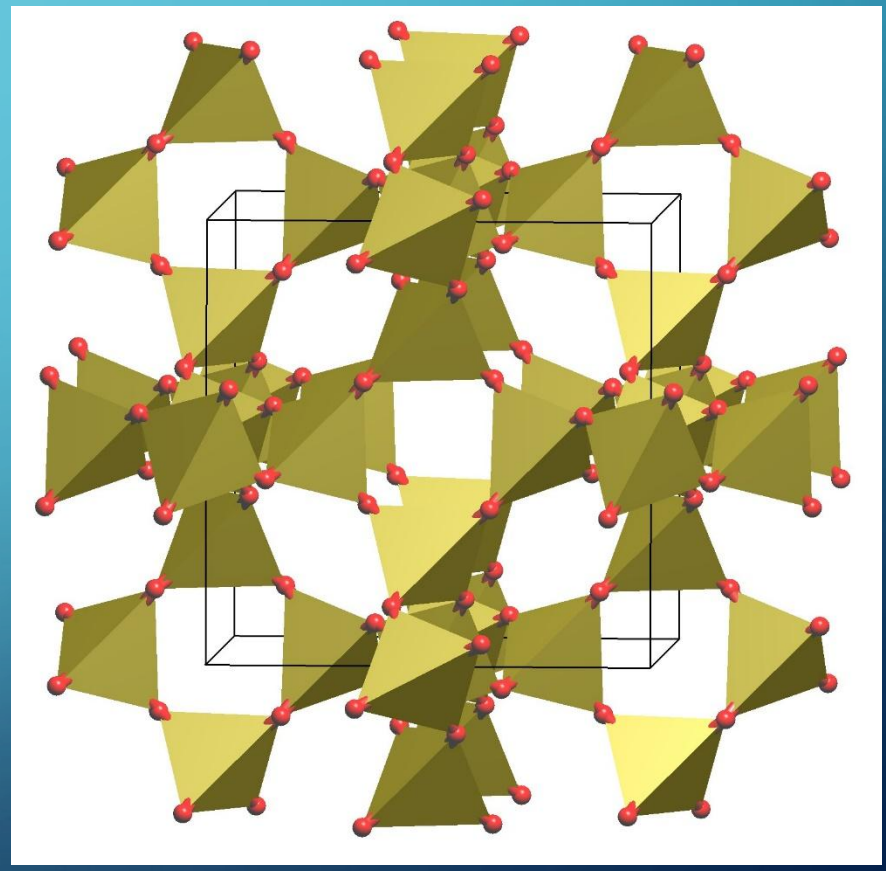
Структура



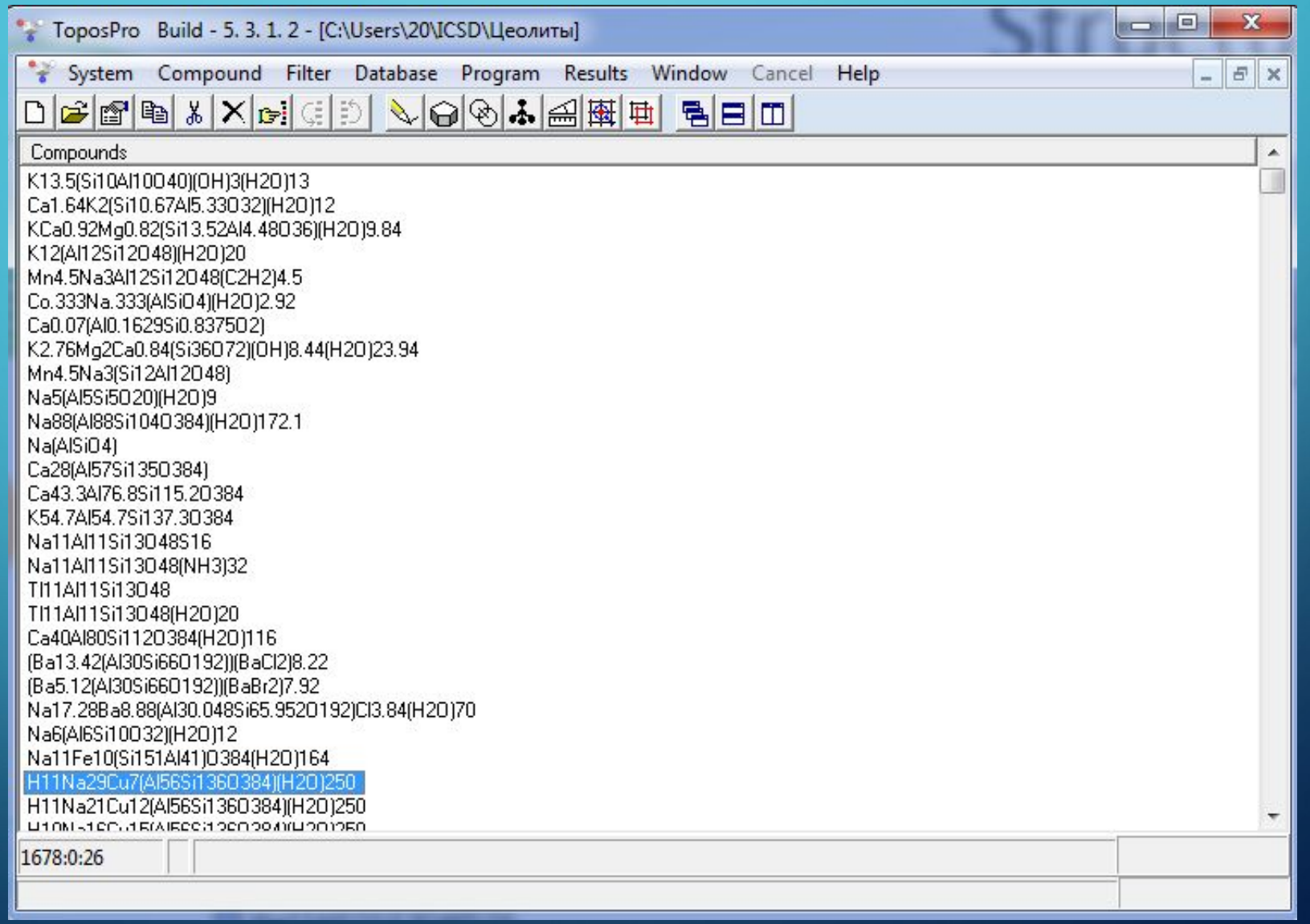
Структура

Si, Al, Be, Mg, P, Ti, Mn, Fe, Zn, Ga, Ge, Co, Ni, Cu

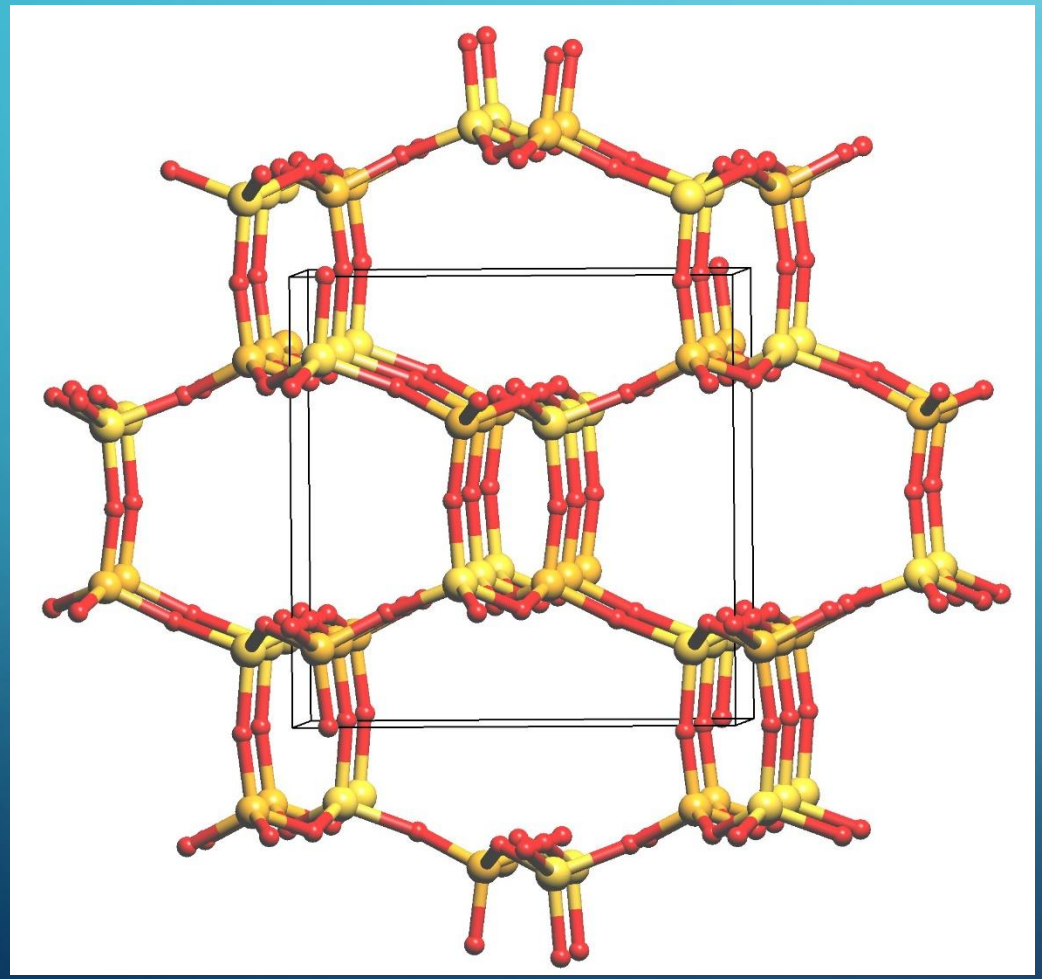


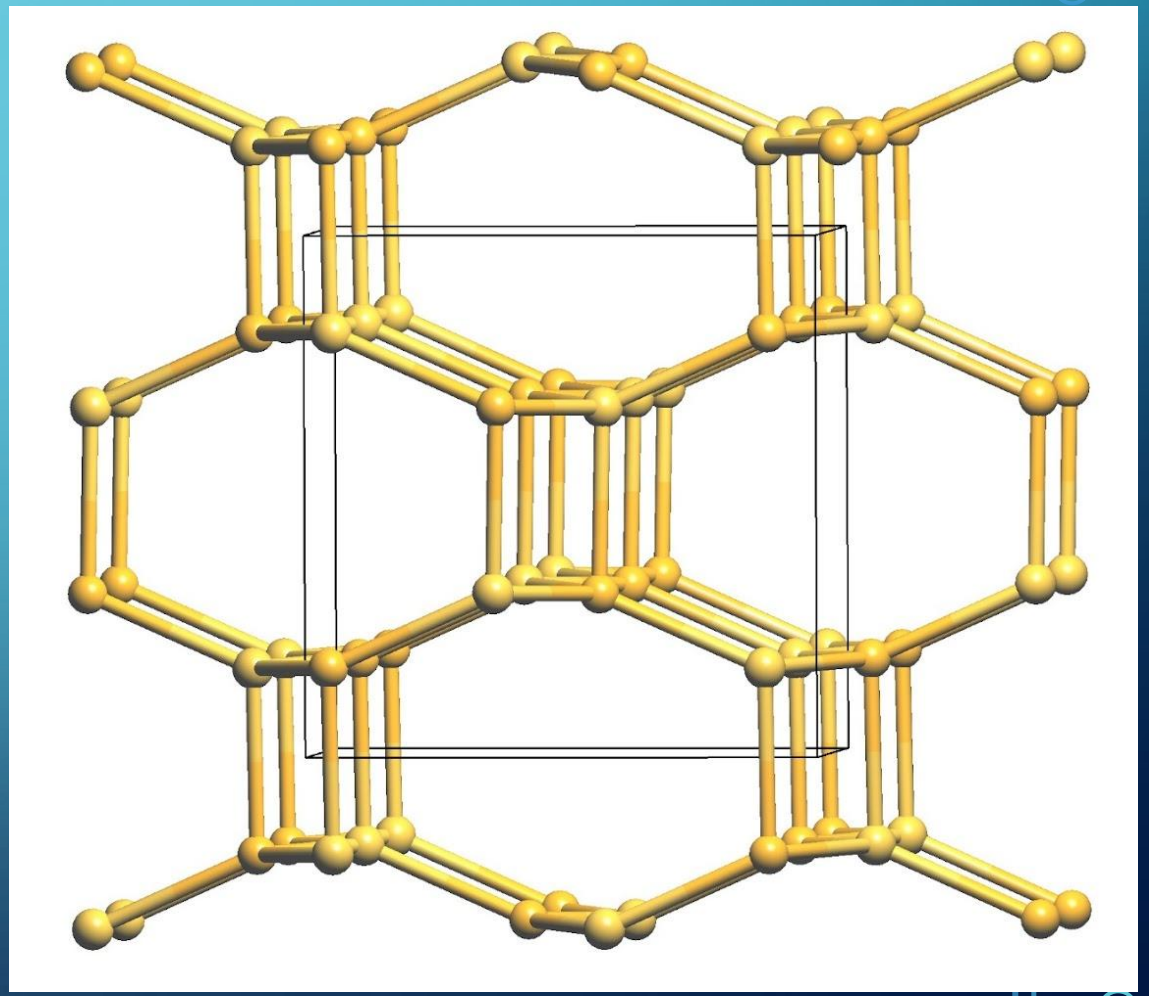


Состав

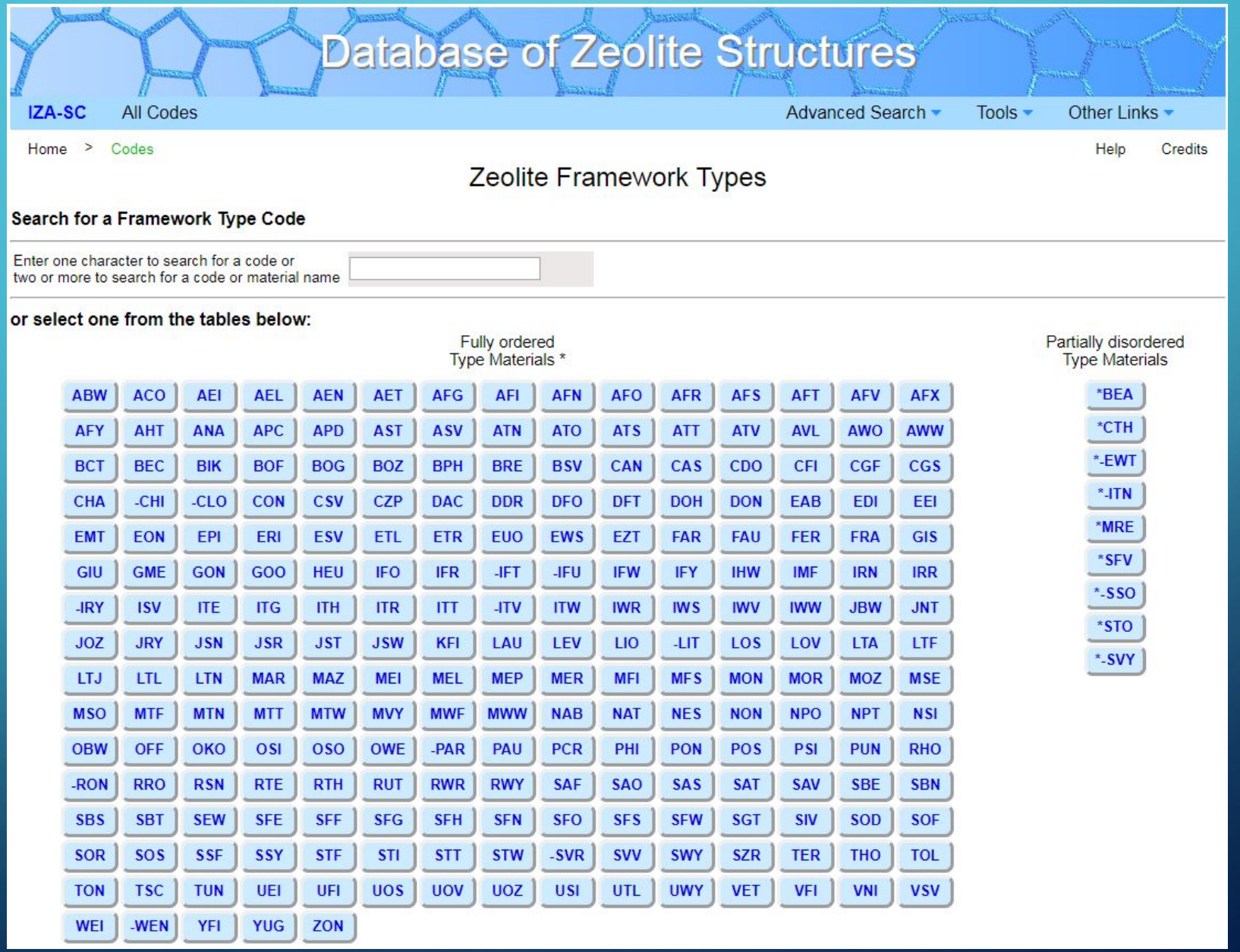

ToposPro Build - 5. 3. 1. 2 - [C:\Users\20\ICSD\Цеолиты]
System Compound Filter Database Program Results Window Cancel Help
Compounds
K13.5(Si10Al10O40)(OH)3(H2O)13
Ca1.64K2(Si10.67Al5.33O32)(H2O)12
KCa0.92Mg0.82(Si13.52Al4.48O36)(H2O)9.84
K12(Al12Si12O48)(H2O)20
Mn4.5Na3Al12Si12O48(C2H2)4.5
Co.333Na.333(AlSiO4)(H2O)2.92
Ca0.07(Al0.1629Si0.8375O2)
K2.76Mg2Ca0.84(Si36O72)(OH)8.44(H2O)23.94
Mn4.5Na3(Si12Al12O48)
Na5(Al5Si5O20)(H2O)9
Na88(Al88Si104O384)(H2O)172.1
Na(AlSiO4)
Ca28(Al57Si135O384)
Ca43.3Al76.8Si115.2O384
K54.7Al54.7Si137.3O384
Na11Al11Si13O48S16
Na11Al11Si13O48(NH3)32
Tl11Al11Si13O48
Tl11Al11Si13O48(H2O)20
Ca40Al80Si112O384(H2O)116
(Ba13.42(Al30Si66O192))(BaCl2)8.22
(Ba5.12(Al30Si66O192))(BaBr2)7.92
Na17.28Ba8.88(Al30.048Si65.952O192)Cl3.84(H2O)70
Na6(Al6Si10O32)(H2O)12
Na11Fe10(Si151Al41)O384(H2O)164
H11Na29Cu7(Al56Si136O384)(H2O)250
H11Na21Cu12(Al56Si136O384)(H2O)250
1678:0:26

3D каркас





http://asia.iza-structure.org



Строительные единицы

Database of Zeolite Structures

IZA-SC | All Codes | Framework | Material | 3D Drawing | Powder Pattern | CIF | PDF | References

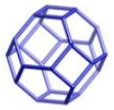
Home » Codes » Framework | Characteristic Units | Help | Credits

Framework Type **FAU**

Framework

Cell Parameters:	cubic	F d -3 m (# 227)	
	a = 24.3450 Å	*b* = 24.3450 Å	*c* = 24.3450Å
	α = 90.000°	β = 90.000°	γ = 90.000°
	Volume =	14428.8Å^3	
	R_{DLS} =	0.0009	
Framework density (FD_{Si}):	13.3 T/1000 Å^3		
Topological density:	TD_{10} = 579	TD = 0.476190	
Ring sizes (# T-atoms):	12 6 4		
Channel dimensionality:	Topological (pore opening > 6-ring): 3-dimensional		
Maximum diameter of a sphere:			
that can be included	11.24 Å		
that can diffuse along	a: 7.35 Å	b: 7.35 Å	c: 7.35 Å
Accessible volume:	27.42 %		
Secondary Building Units:	6-6 or 6-2 or 6 or 4-2 or 1-4-1 or 4		
Composite Building Units:			

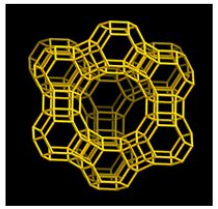
d6r (t-hpr)



sod (t-toc)

Natural Tiling *t-fau* *t-hpr* *t-toc*

Framework images
(click on icon for larger image)



Viewed along [111]

viewed along [110]

Polyhedral model viewed along [110]

an 'artist impression' of a catalytic reaction

Year code assigned 1978
Data last updated Jul 1, 2007

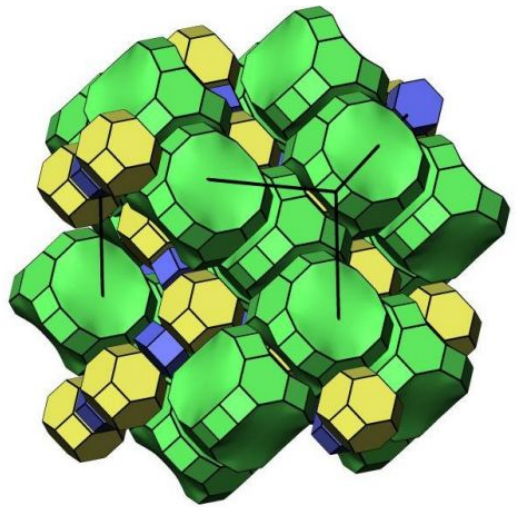
FAU $Fd\bar{3}m$ — $2[4^6.6^2]+[4^6.6^8]+[4^{18}.6^4.12^4]$ — **1 4 5 3**

TILES

Face symbol:	$[4^6.6^2]$	$[4^6.6^8]$	$[4^{18}.6^4.12^4]$
			
V, E, F:	(12, 18, 8)	(24, 36, 14)	(48, 72, 26)
Symmetry:	$\bar{3}m$	$\bar{4}3m$	$\bar{4}3m$
Wyckoff:	16*c*	8*a*	8*b*
Label:	t-hpr	t-toc	t-fau

Special features: ***simple***

TILING



ZSM-5

Zeolite
Socony
Mobil-five

Database of Zeolite Structures

IZA-SC | All Codes | Framework | Material | 3D Drawing | Powder Pattern | CIF | PDF | References

Home » Codes » Type Material | Characteristic Units | Help | Credits

Framework Type **MFI**

Type Material

Material Name: ZSM-5

Chemical Formula§: $|Na^{+}_{n}(H_2O)_{16}|[Al_nSi_{96-n}O_{192}]$-**MFI**, $n < 27$

Unit Cell§: orthorhombic *P n m a (# 62)*

$a' = 20.0700$Å $b' = 19.9200$Å $c' = 13.4200$Å

$\alpha' = 90.000°$ $\beta' = 90.000°$ $\gamma' = 90.000°$

Framework density: 17.9 T/1000 Å^3

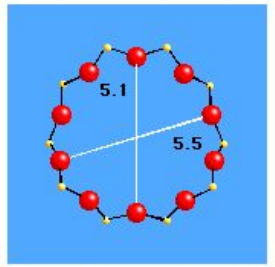
Channels: {[100] **10** 5.1 x 5.5 <-> [010] **10** 5.3 x 5.6}***

Dimensionality

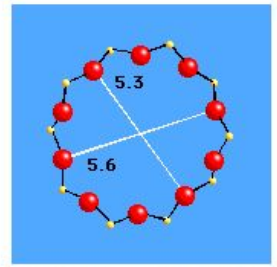
Sorption (molecular cross section > 3.4Å): 3-dimensional

Topological (pore opening > 6-ring): 3-dimensional

Limiting Rings



10-ring viewed along [100]



10-ring viewed along [010]

References:

Kokotailo, G.T., Lawton, S.L., Olson, D.H. and Meier, W.M.
"Structure of synthetic zeolite ZSM-5"
Nature, **272**, 437-438 (1978)

§ Olson, D.H., Kokotailo, G.T., Lawton, S.L. and Meier, W.M.
"Crystal Structure and Structure-Related Properties of ZSM-5"
J. Phys. Chem., **85**, 2238-2243 (1981)

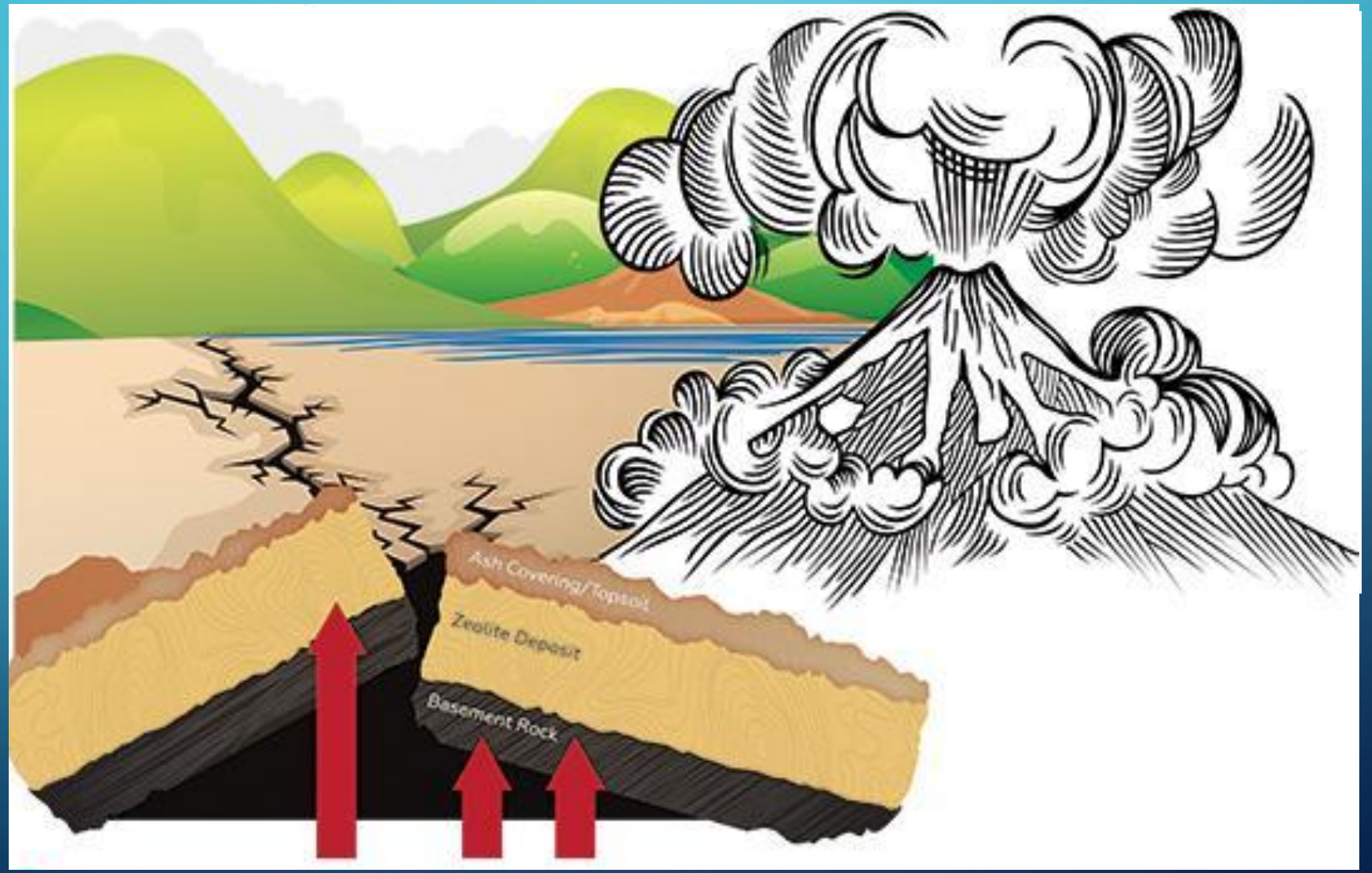
van Koningsveld, H., van Bekkum, H. and Jansen, J.C.
"On the location and disorder of the tetrapropylammonium (TPA) ion in zeolite ZSM-5 with improved framework accuracy"
Acta Crystallogr., **B43**, 127-132 (1987)

Name and Code derivation:

Zeolite Socony Mobil - five
→ ZSM-5 (five)
→ **MFI**

§ *Chemical Formula and Unit Cell taken from the reference marked with this sign*

Цеолиты: образование



Цеолиты: месторождения

Натуральные цеолиты

анальцим

шабазит

гейландит

клиноптилолит

натролит

содалит

стильбит

филипсит

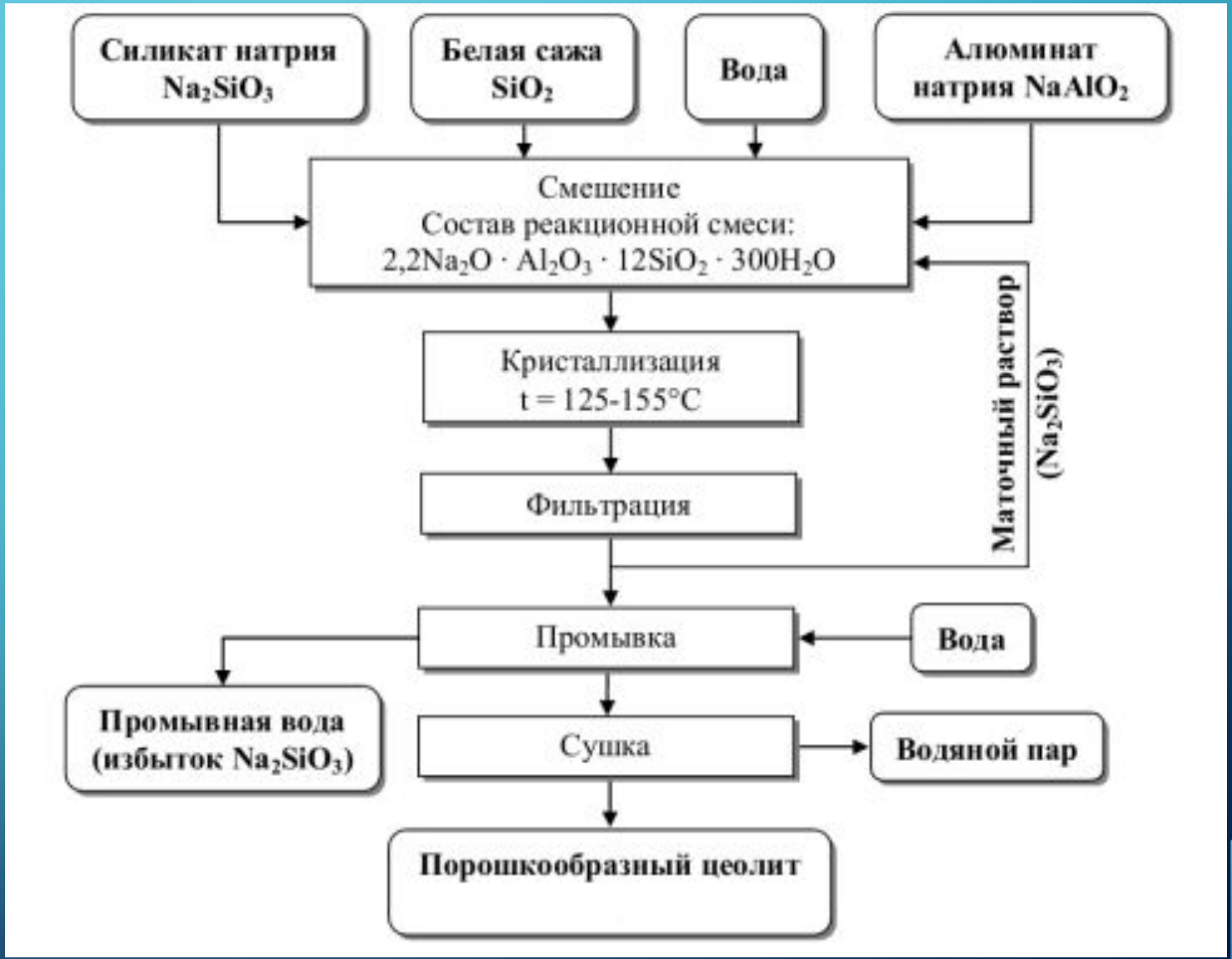
Применение:строительство

4 000 000 т

2 500 000 т

Цеолиты: синтез

- Концентрации растворов
- pH
- Скорость смешивания
- Время перемешивания
- Температура
- Скорость кристаллизации
- Время кристаллизации

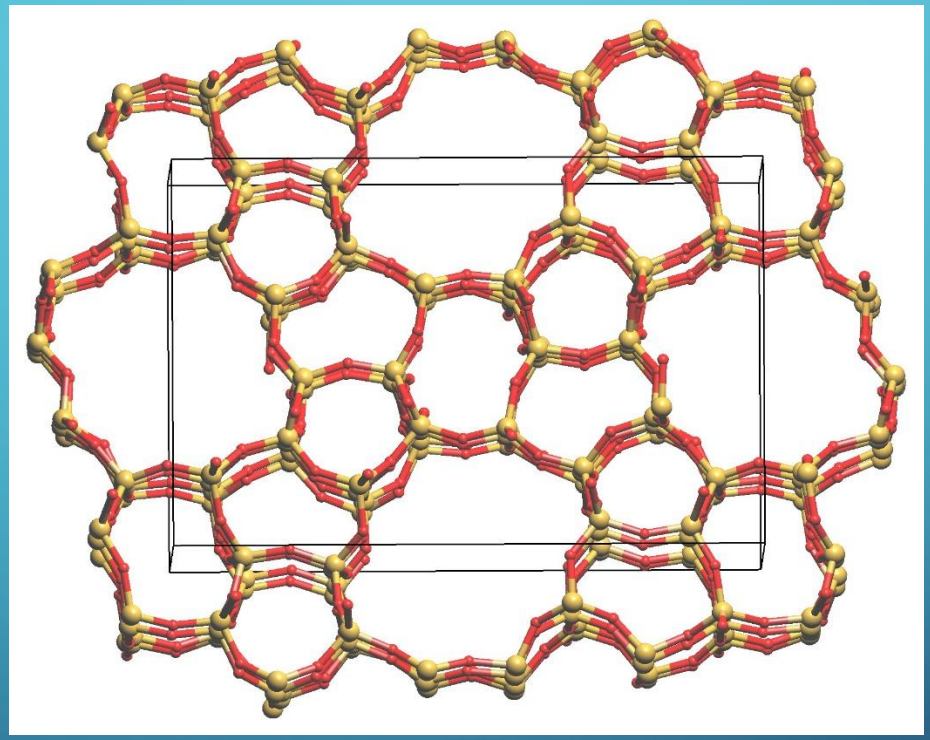


Применение: катализ

ЦеолитY (FAU) 300 000 т

Применение: катализ

Metanol to Gasoline (MTG) Process

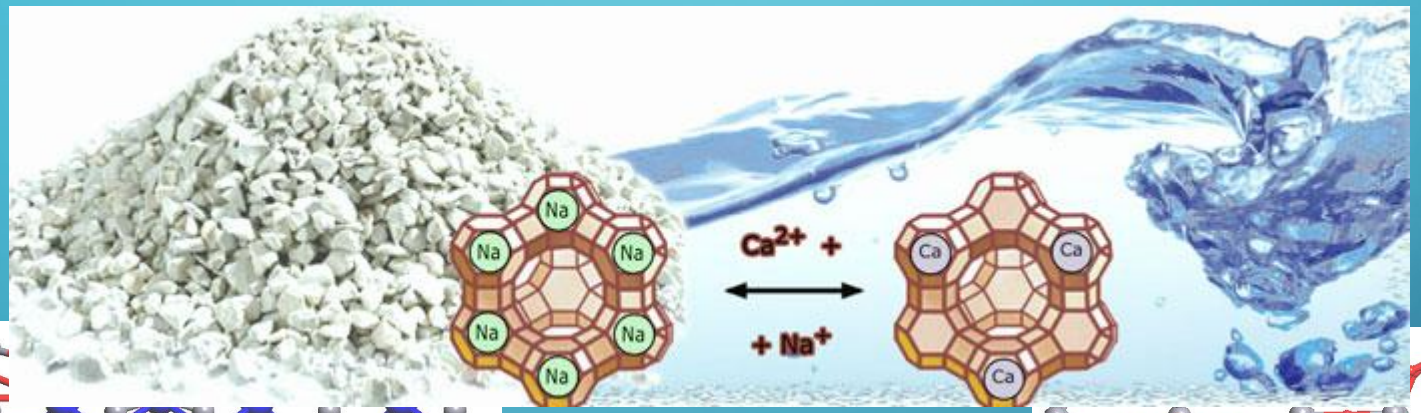


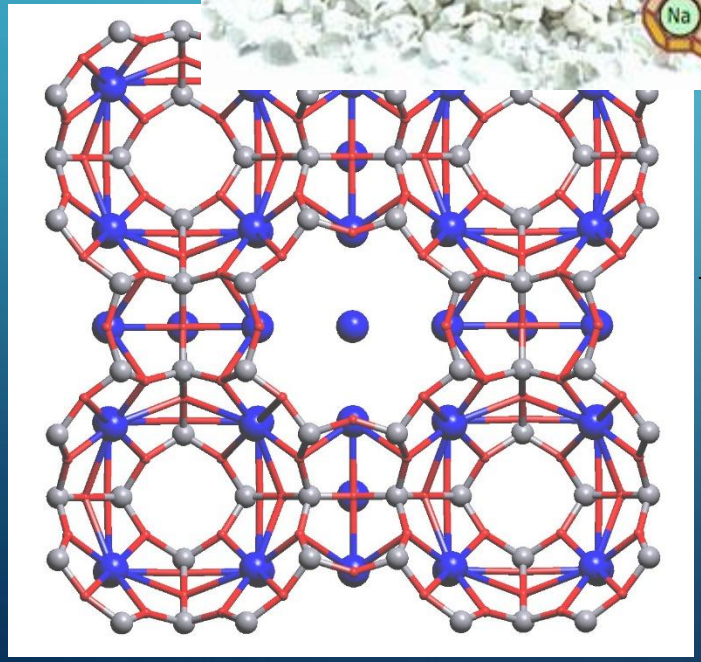
H-ZSM-5
MFI

«Производство полимеров» поли-пара-ксилилен

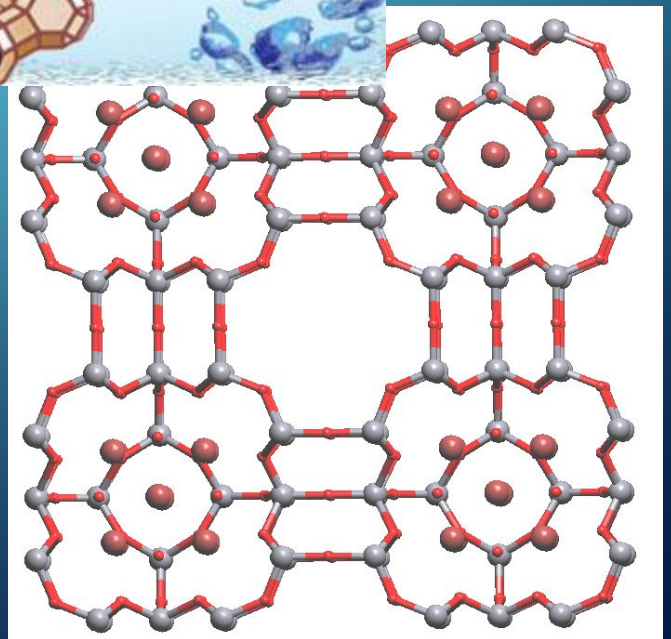
Применение: катионообмен

Цеолит A (LTA)
1,400 000 т





Ca^{2+}, Mg^{2+}, Pb^{2+}, Cd^{2+}, Zn^{2+}

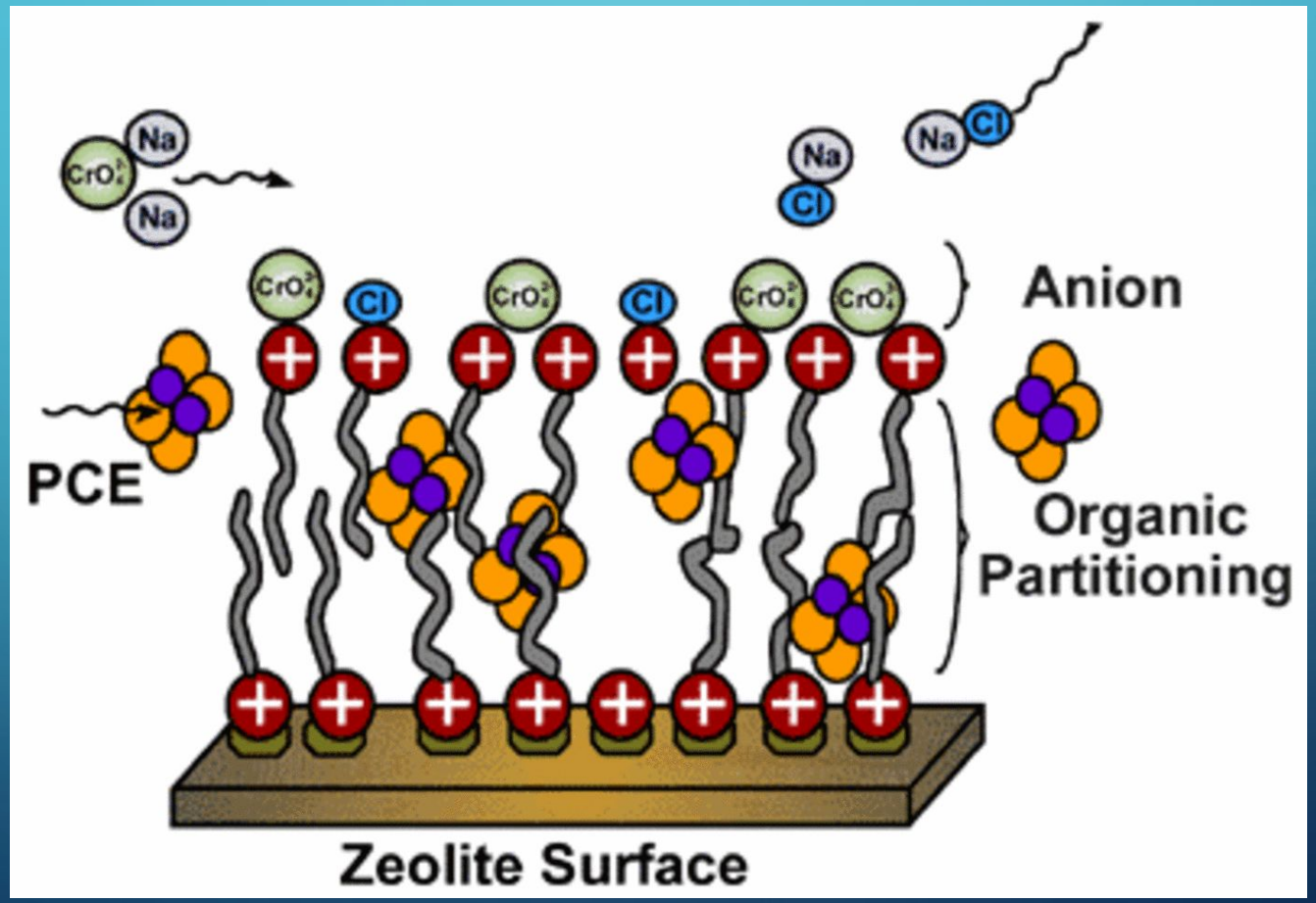


Применение: катионообмен

Клиноптилолит
(HEU)
500 000 т
^{134}Cs, ^{137}Cs, ^{90}Sr

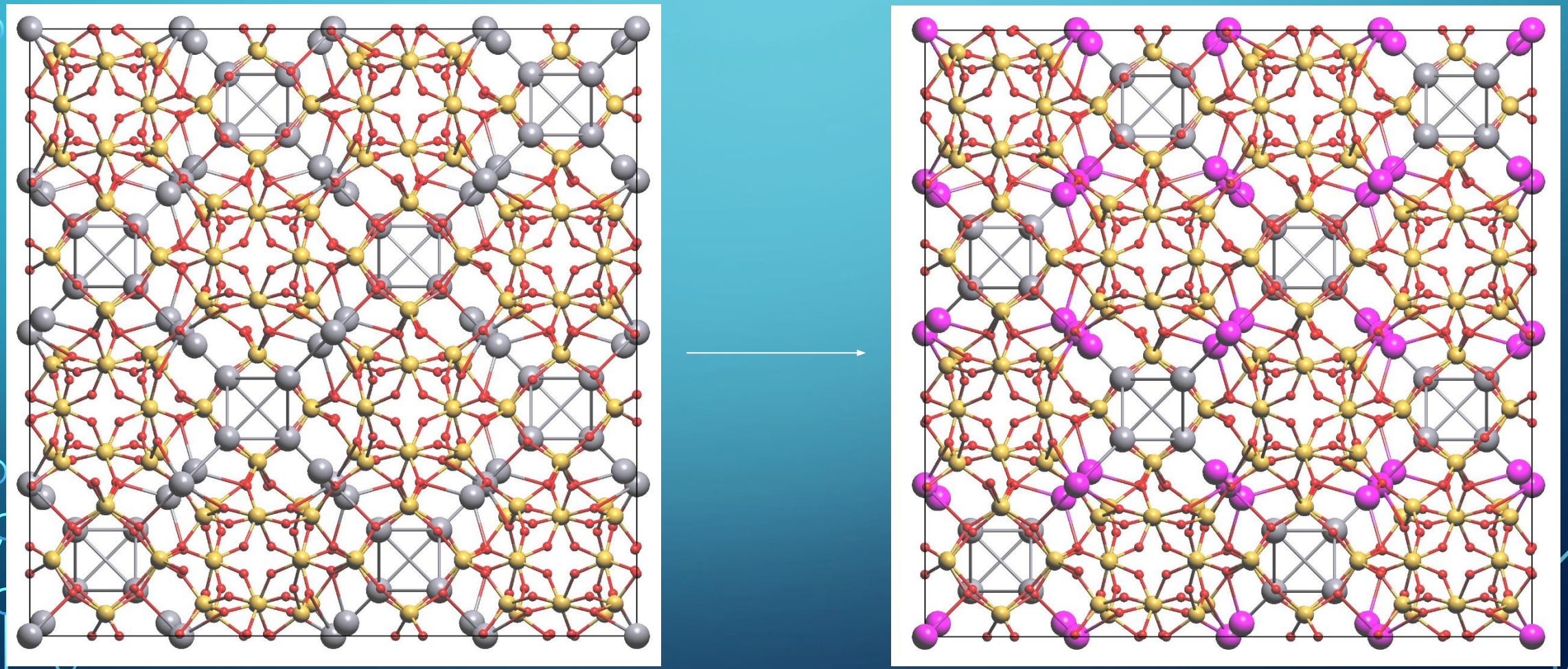
Применение: адсорбция

Клиноптилолит (HEU)

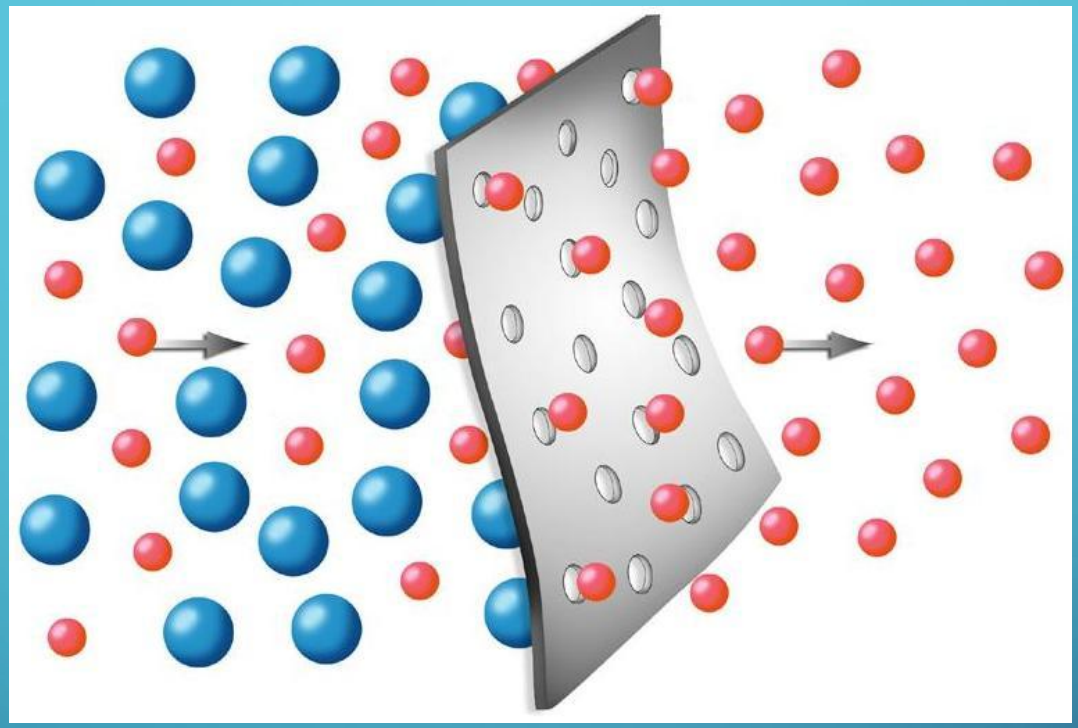


Применение: адсорбция

$$Ag^{+}\text{-Zeolite} + NaI \rightarrow Na^{+}\text{-Zeolite} + AgI\downarrow$$



Применение: молекулярные сита



Осушение

Удаление углеводородов

Разделение газов

Применение: медицина

Применение: сельское хозяйство