



Wrocław University of Technology

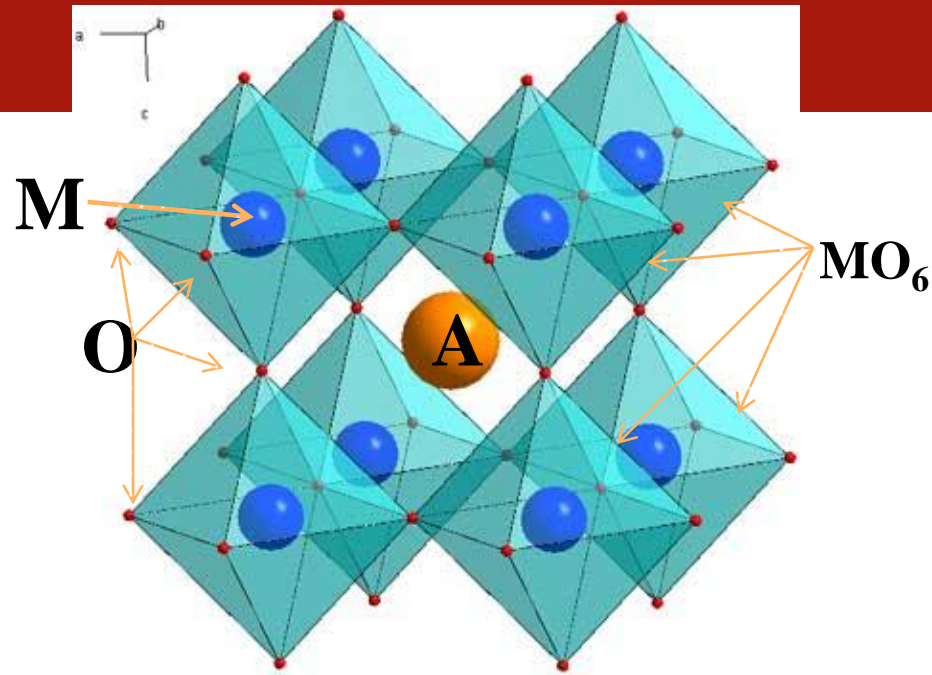
**Związki typu perowskitu – jak
z defektów uczynić zalety...**

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Struktura krystaliczna typu perowskitu

AMX₃



(Na⁺ K⁺ Li⁺ Ag⁺)
(Sb⁺⁵ Bi⁺⁵ Cr⁺⁵ Ta⁺⁵ Nb⁺⁵)



(Mg⁺² Ca⁺² Sr⁺² Ba⁺² Pb⁺² Cd⁺²)
(Sn⁺⁴ Ti⁺⁴ Zr⁺⁴ Pb⁺⁴ Mn⁺⁴ Ce⁺⁴ Mo⁺⁴)



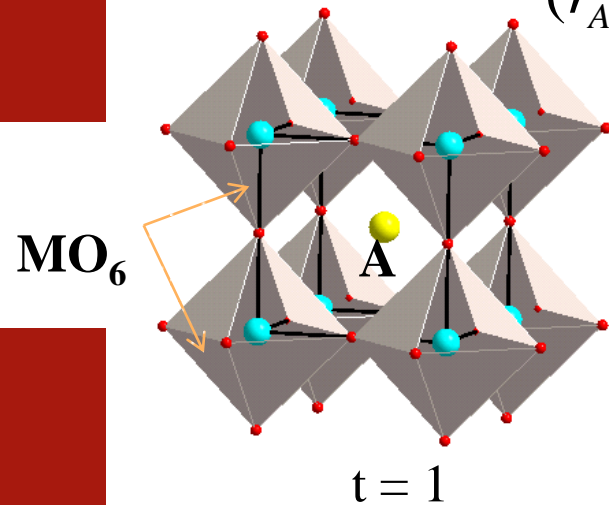
(Y⁺³ Sc⁺³ La⁺³-Lu⁺³)
(Fe⁺³ Cr⁺³ Mn⁺³ Sc⁺³ V⁺³ Al⁺³ In⁺³ Ga⁺³
Co⁺³ Ni⁺³)

Ilość związków perowskitowych jest praktycznie nieograniczona, szczególnie jeśli weźmie się pod uwagę roztwory stałe.

Stabilność struktury perowskitowej

Idealny perowskit
regularny

$$(r_A - r_O) = \sqrt{2}(r_M - r_O)$$

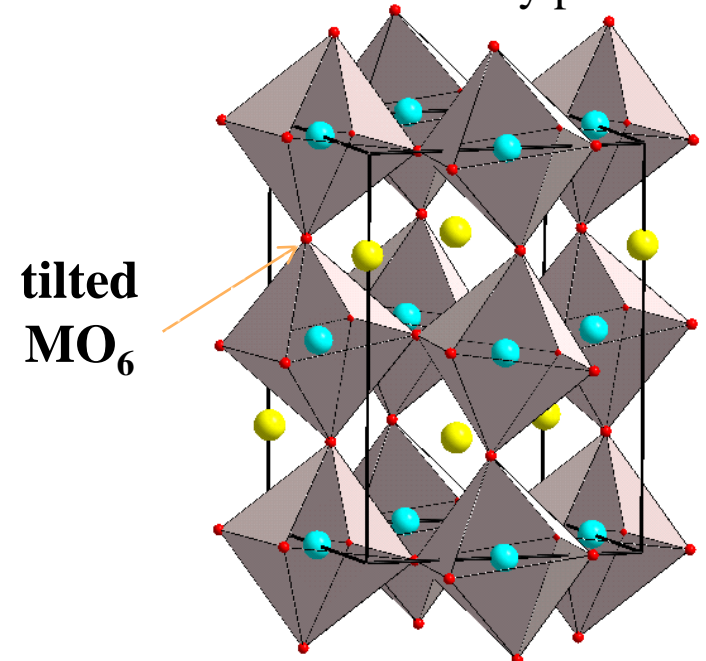


Współczynnik tolerancji: $t = \frac{(r_A - r_O)}{\sqrt{2}(r_M - r_O)}$

r_A, r_M, r_O - promienie jonowe A, M, O.

$$1 > t > 0.75$$

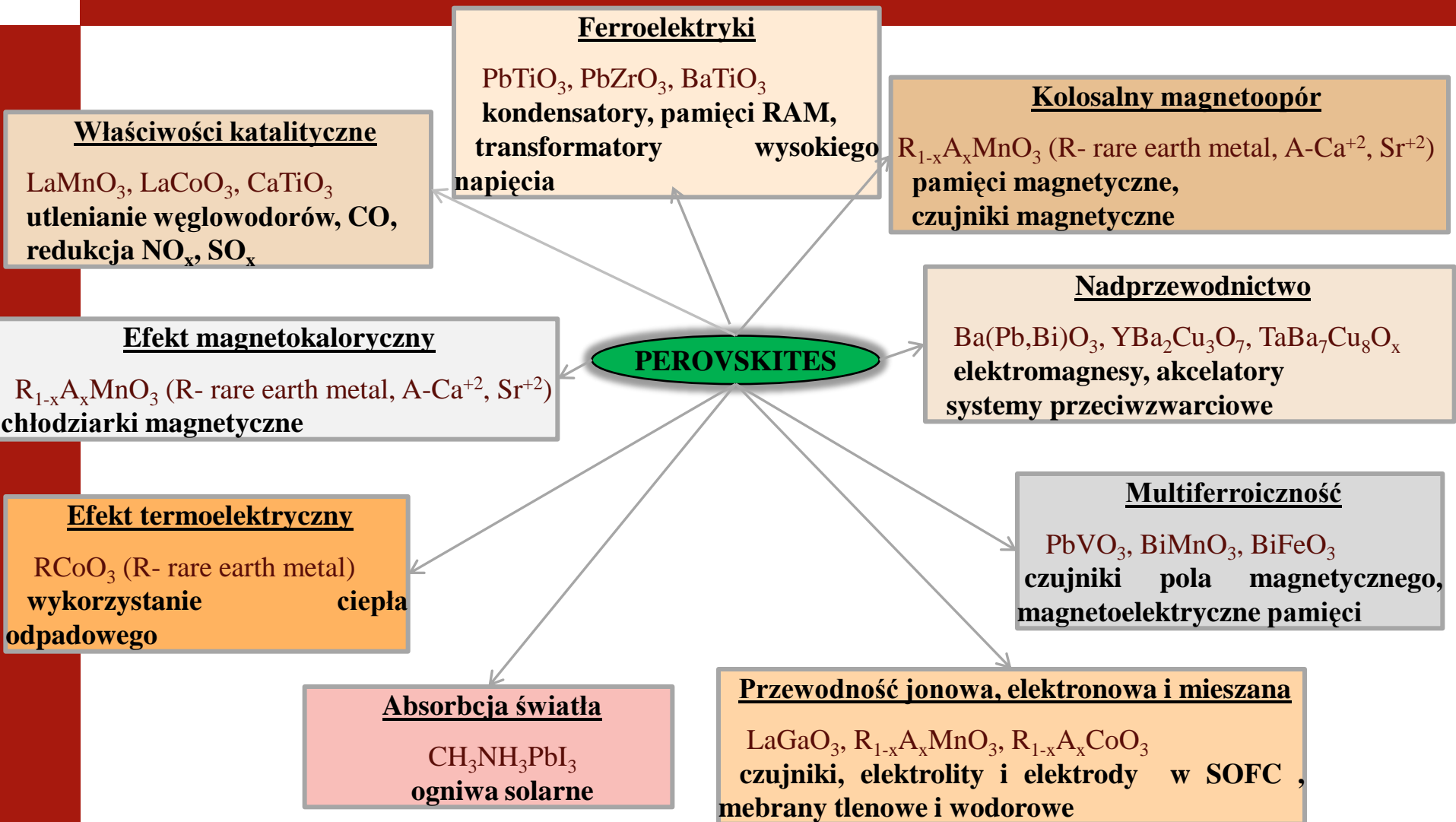
zdeformowany perowskit

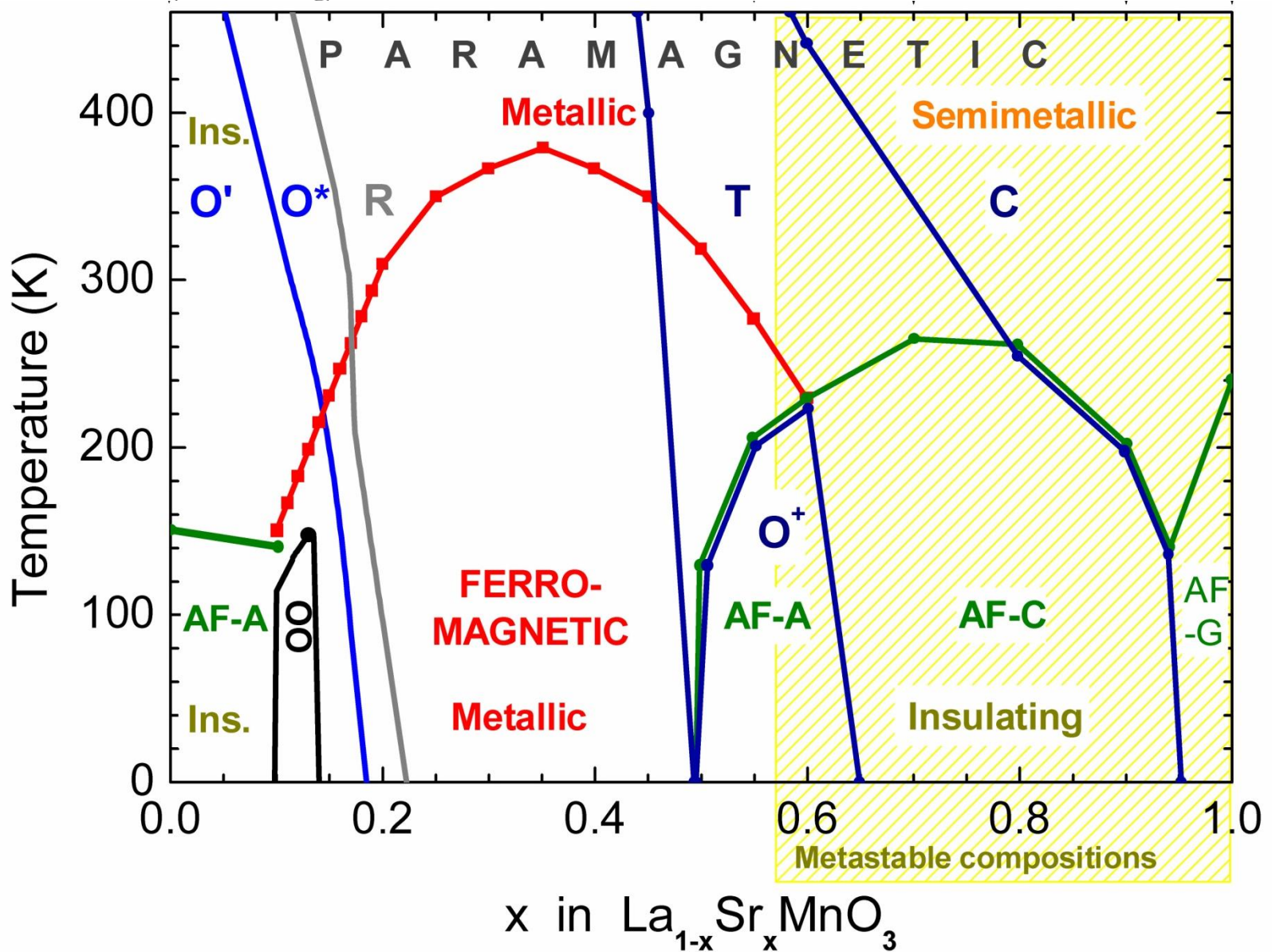


Wiele właściwości perowskitów wykazuje ścisłe powiązanie z dystorsjami sieci krystalicznej.



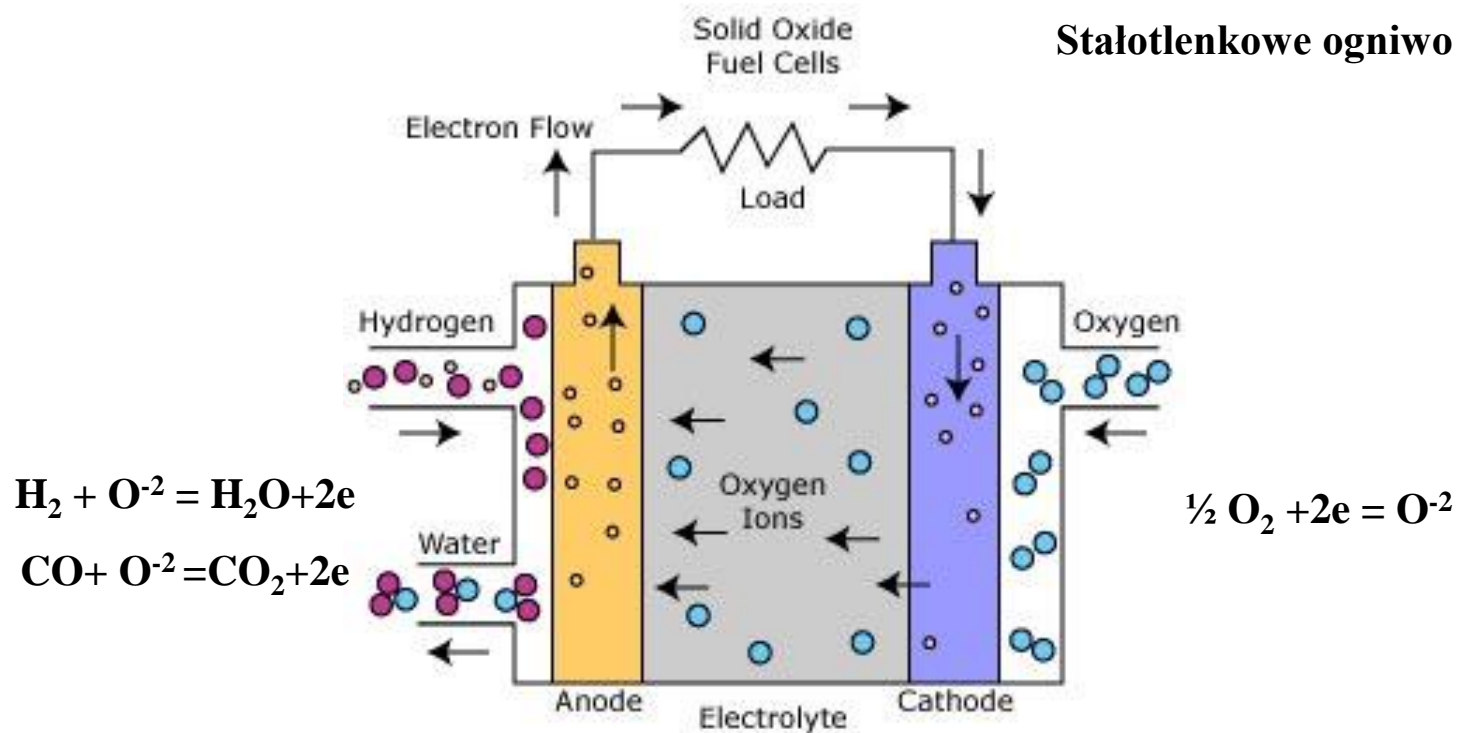
Właściwości fizyczne = zastosowania





Technologie czystej energii

Stalotlenkowe ogniwo paliwowe



Przewodnik mieszany, katalizator

$\text{La}(\text{Sr})\text{Cr}(\text{M})\text{O}_3$ M=Mn, Fe, Co, Ni

Przewodnik jonowy

$\text{La}(\text{Sr})\text{Ga}(\text{Mg})\text{O}_{3-d}$

Przewodnik mieszany, katalizator

$\text{La}(\text{Sr})\text{MnO}_{3-d}$

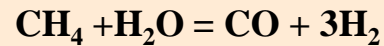
$\text{La}(\text{Sr})\text{CoO}_{3-d}$

$\text{La}(\text{Sr})\text{Fe}(\text{Co})\text{O}_{3-d}$



Produkcja wodoru

Reforming gazu ziemnego:



perowskity = katalizatory
procesu....

LaNiO_3 and $\text{La}_{1-x}\text{Sr}_x\text{NiO}_3$
 SrZrO_3 , $\text{Ni/BaTi}_{0.8}\text{Sn}_{0.2}\text{O}_3$

Syngaz H_2 , CO

Miejsca pozyskiwania biogazu



Wysypisko odpadów



Oczyszczalnia ścieków



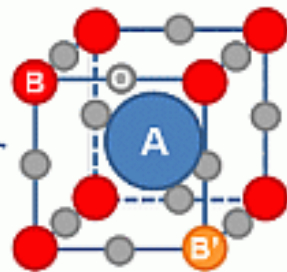
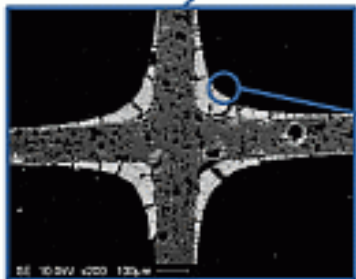
Biogazownia wiejska

Biogaz $\text{CO}_2 + \text{CH}_4$



Skoro mowa o katalizatorach i o czystszej energii...

Three-Way Catalytic Converter



Perovskite-type oxides:

- Redox properties
- Tunability
- Thermal stability
- Self-regenerative properties

Structured catalysts:

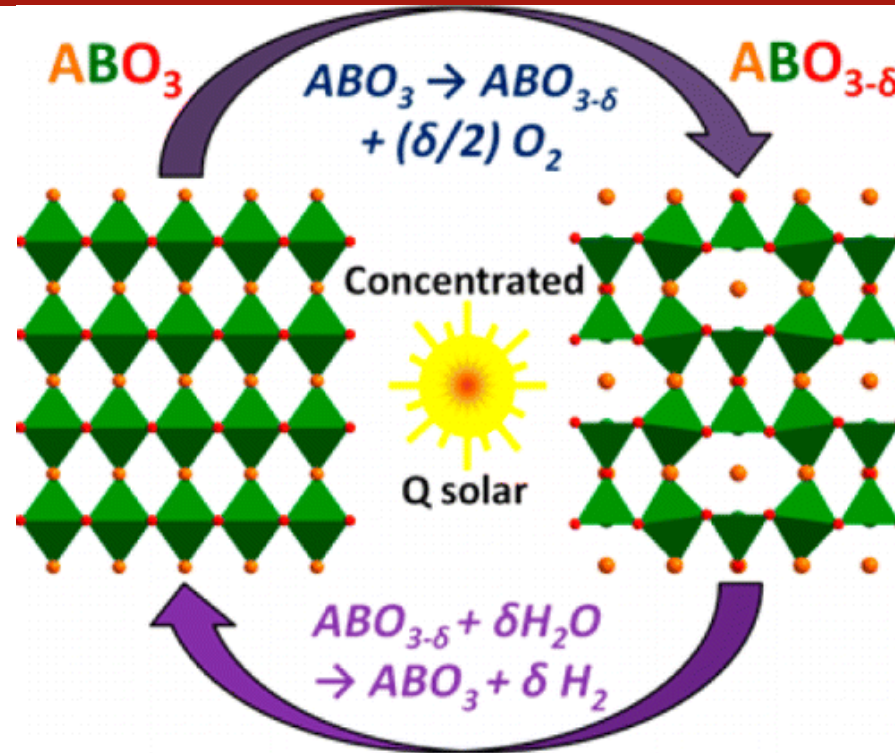
- Extruded catalysts
- Coated catalysts





Produkcja H₂ bezpośrednio z H₂O

La_xSr_{1-x}MO₃ (M = Mn, Co, Fe),
Ba_xSr_{1-x}(Co,Fe)O₃, LaSrCoO₄,
LaSrFeO₄



Termochemiczne reaktory solarne produkcji wodoru- solar thermochemical splitting of H₂O

Również:

Termochemiczne magazyny energii słonecznej - solar Thermal Energy Storage (TES)

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High temperature neutron diffraction studies of PrInO_3 and the measures of perovskite structure distortion

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The crystal structure of PrInO_3 was investigated in the temperature range 303–1123 K by high-resolution neutron-powder diffraction. The PrInO_3 adopts a highly distorted variant of the perovskite structure with the orthorhombic $Pnma$ space group in the whole temperature range investigated. The bond length and bond-angle analysis revealed a very slow tendency to decrease structural distortion with increasing temperature. Comparison of different parameters quantifying perovskite structure distortion calculated for PrInO_3 and the similar PrAlO_3 and PrGaO_3 shows the advantage of using the tolerance factor t_{12} calculated for the 12-fold coordinated Pr by geometrical averaging of the individual interatomic distances. An additional advantage of the tolerance factor method results from the possibility of extending it to predict the average structural distortion and the geometrical stability of the perovskites at various temperatures once the accurate dependence of $t(x, T, d)$ on the composition, temperature and oxygen content is found. By comparing PrInO_3 with several AMO_3 perovskites containing ions in the fixed oxidation state on the A and M crystal sites it was found that structural distortion and the tolerance factor t_{12} for PrInO_3 are consistent with the empirical thermal expansion coefficient based on the bond strength calculation [R. M. Hazen, and C. T. Prewitt, *Am. Mineral.*, 1977, **62**(3–4), 309]. In contrast to perovskites AMO_{3-d} con-