Creating a Redox Materials Database for Solar-Thermochemical Air Separation and Fuels Production

J. Vieten, P. Huck, M. Horton, B. Bulfin, D. Guban, L. Zhu, M. Roeb, K.A. Persson, C. Sattler

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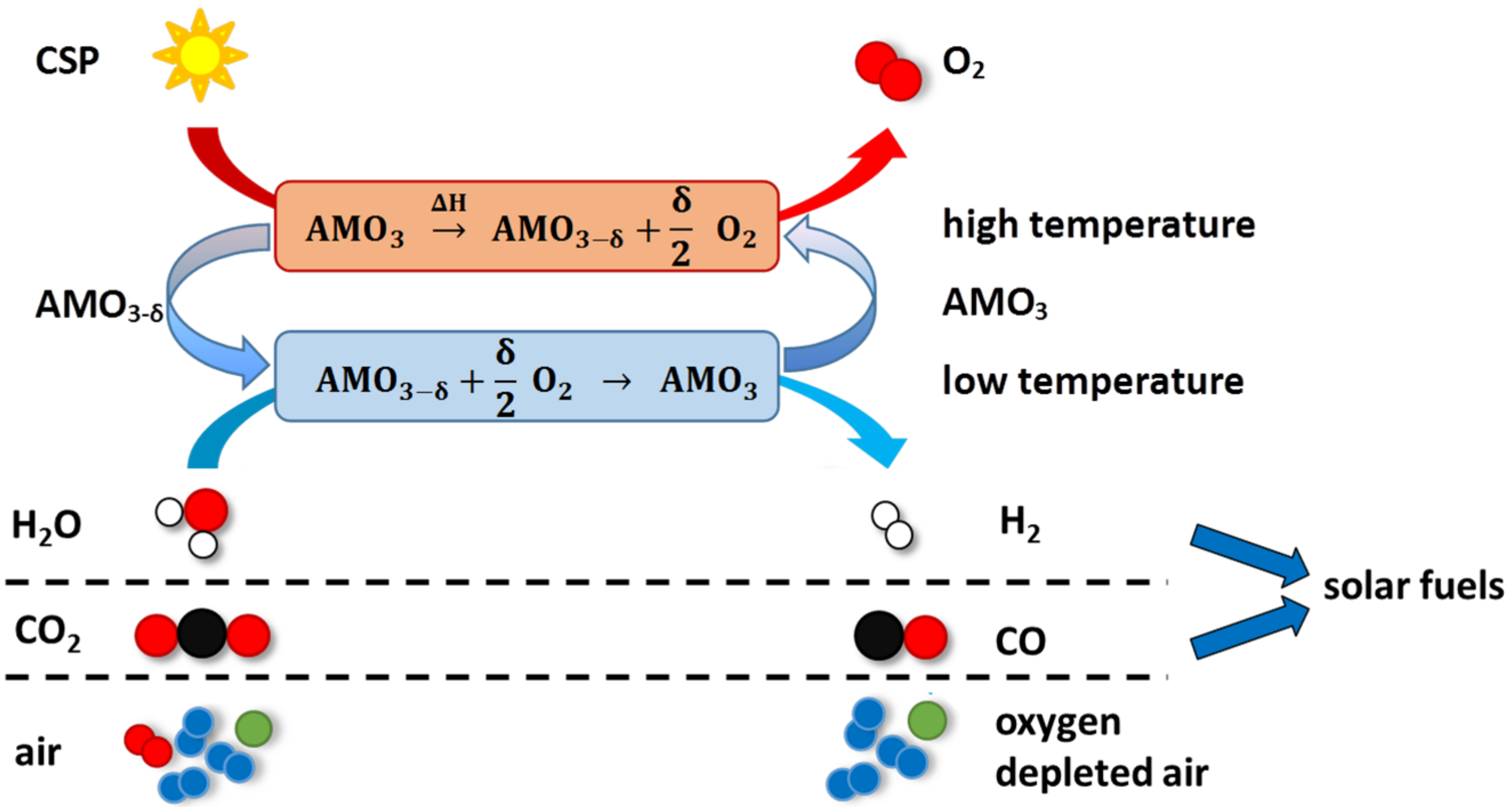
Solar-thermochemical redox cycles

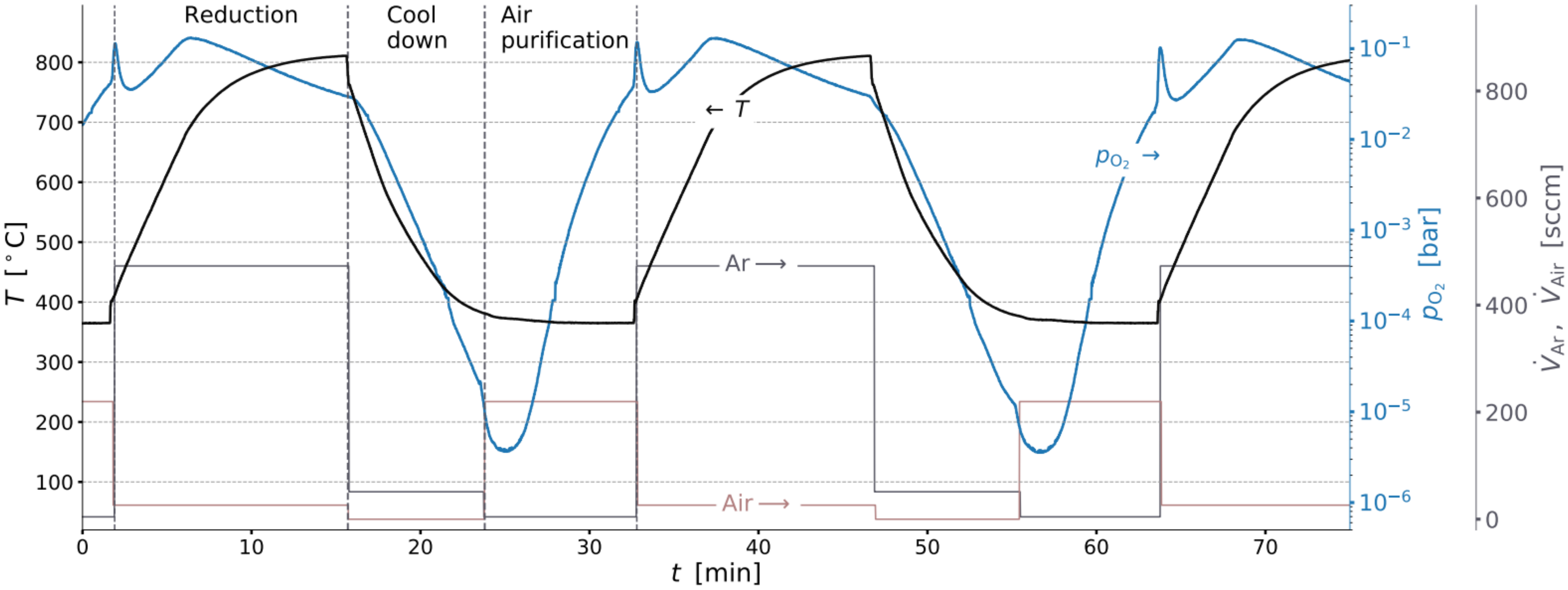


→ nitrogen/oxygen depleted air: application in Haber-Bosch ammonia production

(currently > 1% of world primary energy consumption[1])

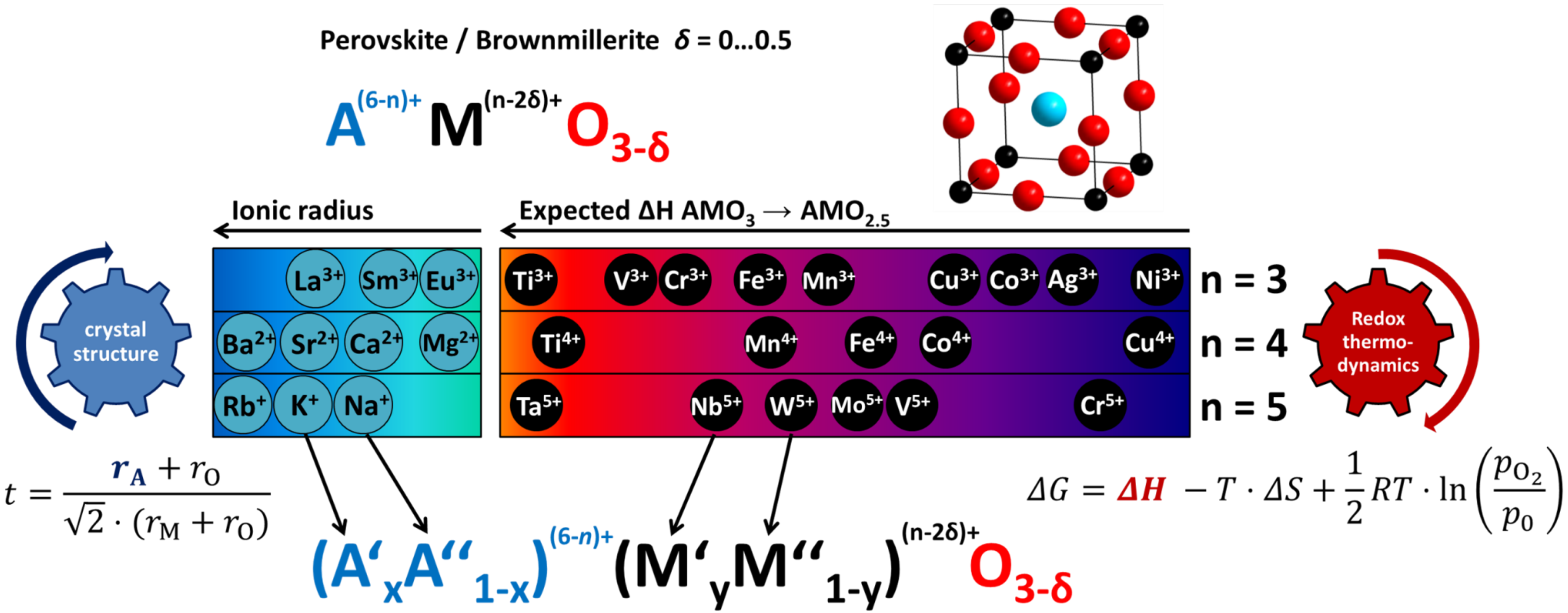
[1] Erisman, J. W.; Sutton, M. A.; Galloway, J.; Klimont, Z.; Winiwarter, W., How a century of ammonia synthesis changed the world. Nature Geosci 2008, 1, (10), 636-639.
[2] Vieten, J.; Bulfin, B.; Starr David, E.; Hariki, A.; de Groot Frank, M. F.; Azarpira, A.; Zachäus, C.; Hävecker, M.; Skorupska, K.; Knoblauch, N.; Schmücker, M.; Roeb, M.; Sattler, C. Redox behavior of solid solutions in the SrFe1-xCuxO3-δ system for application in thermochemical oxygen storage and air separation. Energy Technology 2018, 0 (ja)

Example: Laboratory scale air separation with $SrFeO_{3-\delta}$



[3] Bulfin, B.; Lapp, J.; Guban, D.; Vieten, J.; Richter, S.; Brendelberger, S.; Roeb, M.; Sattler, C. Thermochemical air separation and selective oxygen pumping with an SrFeO3 redox cycle. submitted 2018.

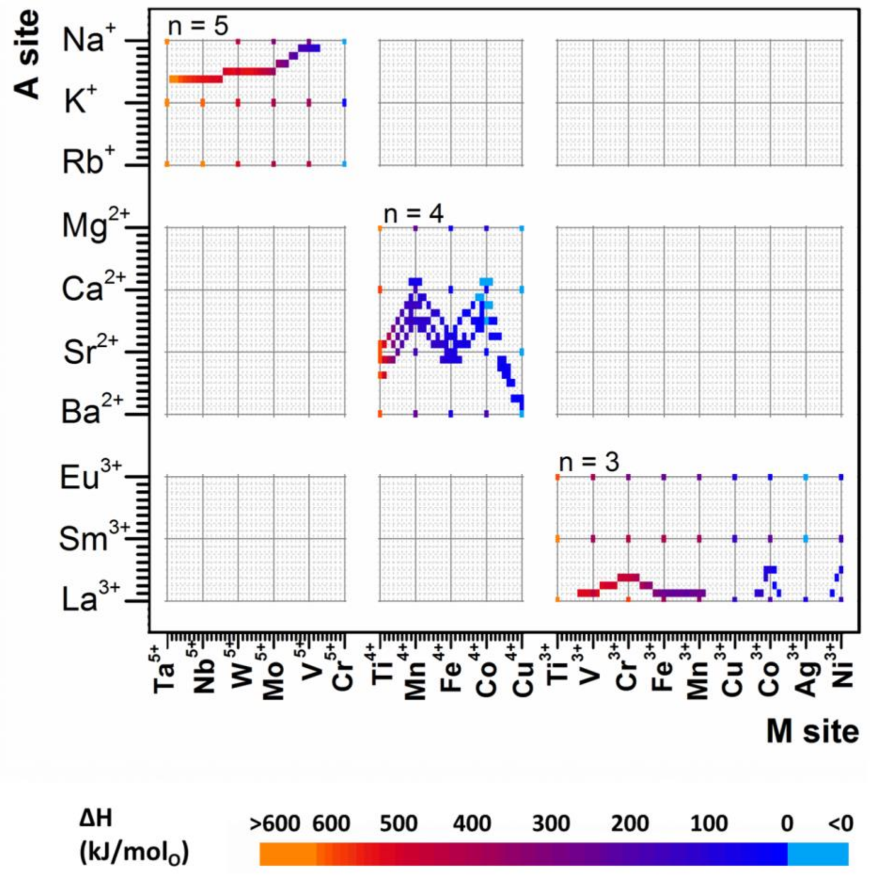
Designing perovskite solid solutions



[4] Vieten, J.; Bulfin, B.; Huck, P.; Horton, M.; Guban, D.; Zhu, L.; Persson, K.; Roeb, M.; Sattler, C., Materials design of perovskite solid solutions for thermochemical applications. prepared 2018.

DFT results – redox enthalpies for > 240 perovskite-brownmillerite pairs

$$2\,(A'_xA''_{1-x})(M'_yM''_{1-y})O_3 \rightarrow 2\,(A'_xA''_{1-x})(M'_yM''_{1-y})O_{2.5} + 0.5\,O_2$$



- Wide range of redox enthalpies spanned: -340 to 706 kJ/mol$_O$
- Over 50 % in the range from 50 to 400 kJ/mol$_O$

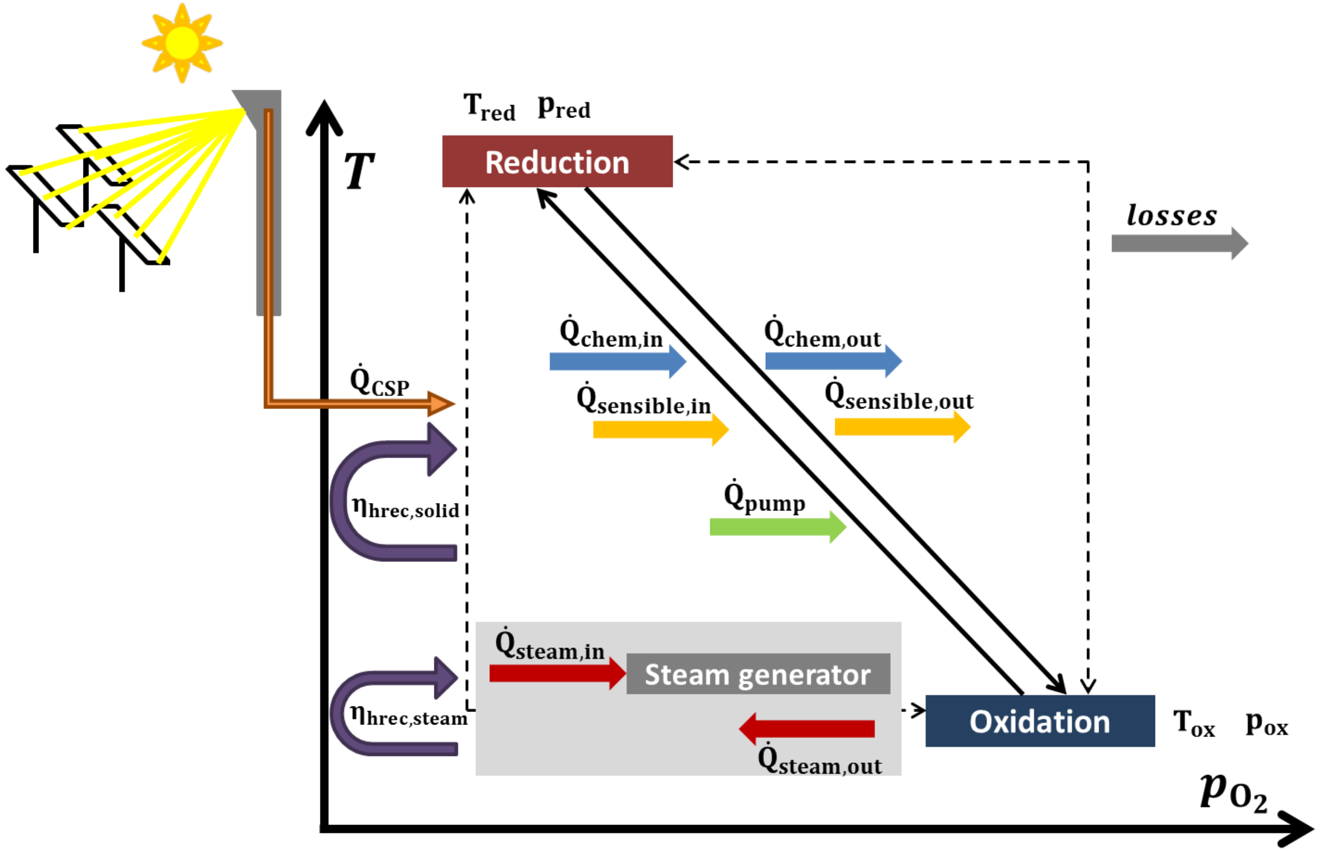
ranked list:

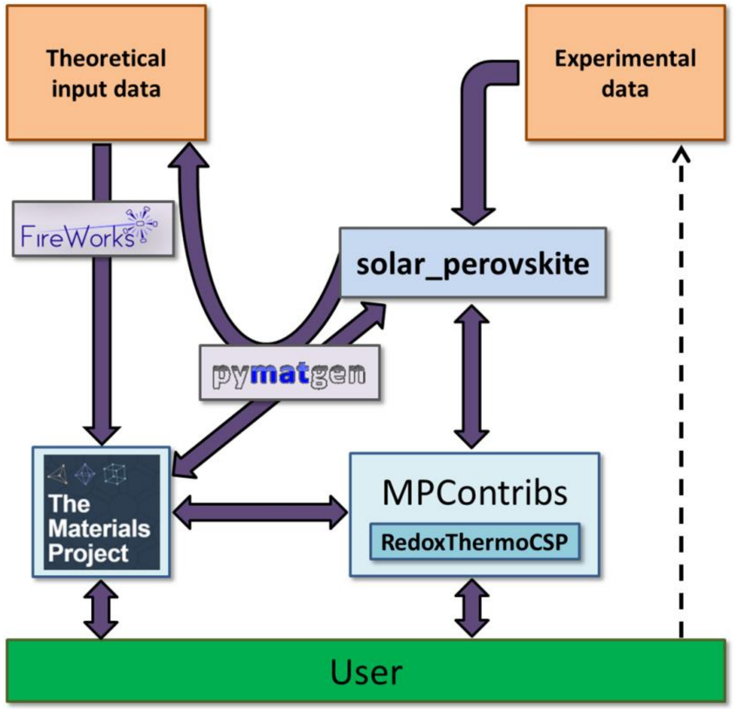
Redox Material	*n*	*t*	ΔH (kJ/mol$_O$)
$Ca_{0.875}Sr_{0.125}Mn_{0.75}Fe_{0.25}O_{3-\delta}$	4	0.994	101.07
$Ca_{0.875}Sr_{0.125}Mn_{0.875}Fe_{0.125}O_{3-\delta}$	4	0.997	102.62
$Na_{0.875}K_{0.125}V_{0.75}Cr_{0.25}O_{3-\delta}$	5	1.025	102.72
$EuCuO_{3-\delta}$	3	0.879	105.30
$Ca_{0.75}Sr_{0.25}Mn_{0.625}Fe_{0.375}O_{3-\delta}$	4	0.995	105.69
$SrMn_{0.125}Fe_{0.875}O_{3-\delta}$	4	1.009	105.84
$Sm_{0.375}La_{0.625}Cu_{0.125}Co_{0.875}O_{3-\delta}$	3	0.943	106.73

average distance between two consecutive entries: 2.5 kJ/mol$_O$

[4] Vieten, J.; Bulfin, B.; Huck, P.; Horton, M.; Guban, D.; Zhu, L.; Persson, K.; Roeb, M.; Sattler, C., Materials design of perovskite solid solutions for thermochemical applications. prepared 2018.

Modelling the redox cycle to rank materials according to their energy demand

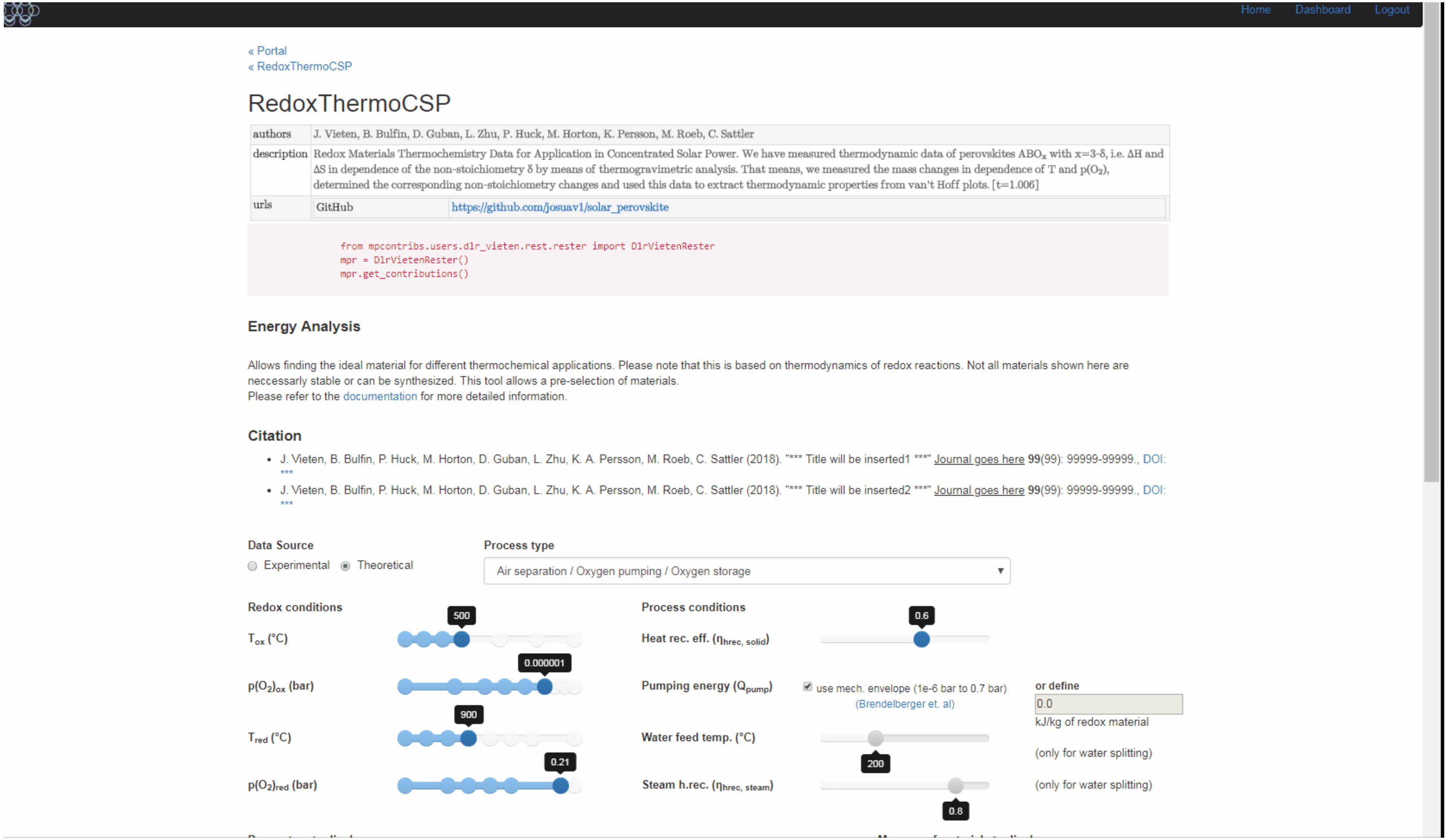




https://materialsproject.org/mpcontribs

[5] Vieten, J.; Bulfin, B.; Huck, P.; Horton, M.; Guban, D.; Zhu, L.; Persson, K.; Roeb, M.; Sattler, C., Energetic analysis of two-step thermochemical cycles based on perovskite solid solutions. prepared 2018.

Demonstration: RedoxThermoCSP @ Materials Project/MPContribs



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RedoxThermoCSP

authors	J. Vieten, B. Bulfin, D. Guban, L. Zhu, P. Huck, M. Horton, K. Persson, M. Roeb, C. Sattler
description	Redox Materials Thermochemistry Data for Application in Concentrated Solar Power. We have measured thermodynamic data of perovskites ABO_x with x=3-δ, i.e. ΔH and ΔS in dependence of the non-stoichiometry δ by means of thermogravimetric analysis. That means, we measured the mass changes in dependence of T and $p(O_2)$, determined the corresponding non-stoichiometry changes and used this data to extract thermodynamic properties from van't Hoff plots. [t=1.006]
urls	GitHub https://github.com/josuav1/solar_perovskite

```
from mpcontribs.users.dlr_vieten.rest.rester import DlrVietenRester
mpr = DlrVietenRester()
mpr.get_contributions()
```

Energy Analysis

Allows finding the ideal material for different thermochemical applications. Please note that this is based on thermodynamics of redox reactions. Not all materials shown here are neccessarly stable or can be synthesized. This tool allows a pre-selection of materials.
Please refer to the documentation for more detailed information.

Citation

- J. Vieten, B. Bulfin, P. Huck, M. Horton, D. Guban, L. Zhu, K. A. Persson, M. Roeb, C. Sattler (2018). "*** Title will be inserted1 ***" Journal goes here **99**(99): 99999-99999., DOI: ***
- J. Vieten, B. Bulfin, P. Huck, M. Horton, D. Guban, L. Zhu, K. A. Persson, M. Roeb, C. Sattler (2018). "*** Title will be inserted2 ***" Journal goes here **99**(99): 99999-99999., DOI: ***

Data Source
Experimental Theoretical

Process type
Air separation / Oxygen pumping / Oxygen storage

Redox conditions

T_{ox} (°C) 500

$p(O_2)_{ox}$ (bar) 0.000001

T_{red} (°C) 900

$p(O_2)_{red}$ (bar) 0.21

Process conditions

Heat rec. eff. ($\eta_{hrec,\ solid}$) 0.6

Pumping energy (Q_{pump}) use mech. envelope (1e-6 bar to 0.7 bar) (Brendelberger et. al) or define 0.0 kJ/kg of redox material

Water feed temp. (°C) 200 (only for water splitting)

Steam h.rec. ($\eta_{hrec,\ steam}$) 0.8 (only for water splitting)

Thank you for your attention!