

## Supplemental Information

# Key Developments in Magnesiothermic Reduction of Silica: Insights into Reactivity and Future Prospects

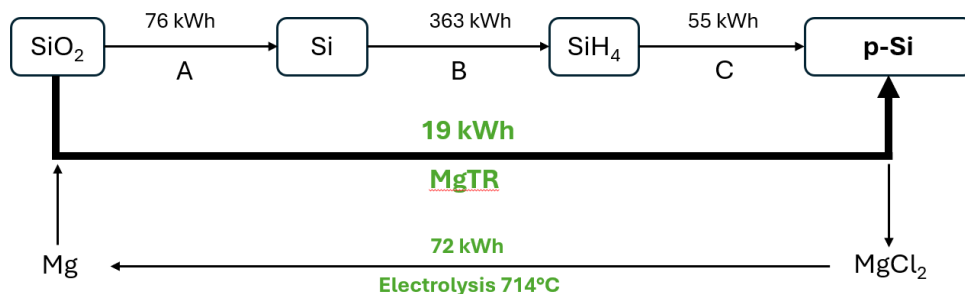
Maximilian Yan<sup>a,b,‡</sup>, Sarah Martell<sup>a,‡</sup>, Siddharth V. Patwardhan<sup>b</sup>, and Mita Dasog<sup>a\*</sup>

<sup>a</sup>*Department of Chemistry, Dalhousie University, 6243 Alumni Crescent, Halifax, NS B3H4R2, Canada.*

<sup>b</sup>*Department of Chemical and Biological Engineering, The University of Sheffield, Mappin Street, Sheffield S1 3JD, United Kingdom.*

\*Corresponding author: [mita.dasog@dal.ca](mailto:mita.dasog@dal.ca)

‡*These authors contributed equally to the work and their names can be listed in any order.*



**Figure S1:** Schematic showing high volume production routes to making porous Si, and the energy requirement of each step, normalised to 1 kg of Si.

**Table S1:** Chemical process occurring in each step described in Figure S1, along with associated energy cost and reference source.

Step	Process	Energy cost (kWh/kg Si)	doi
A	Carbothermal reduction	76	<a href="https://doi.org/10.1016/j.jpowsour.2023.233720">https://doi.org/10.1016/j.jpowsour.2023.233720</a> *
B	Silane production	363	<a href="https://doi.org/10.1016/j.resconrec.2012.10.002">https://doi.org/10.1016/j.resconrec.2012.10.002</a>
C	Siemens process	55	<a href="https://doi.org/10.1016/j.applthermaleng.2021.117522">https://doi.org/10.1016/j.applthermaleng.2021.117522</a> <a href="https://doi.org/10.1016/j.jcryspro.2014.05.020">https://doi.org/10.1016/j.jcryspro.2014.05.020</a>
MgTR	Magnesiothermic reduction	19	<a href="https://doi.org/10.1016/j.jpowsour.2023.233720">https://doi.org/10.1016/j.jpowsour.2023.233720</a> *
Electrolysis	Molten salt electrolysis	72	Calculated here, see Table S3

\*Energy cost was calculated with the model used in our previous work<sup>1</sup> under the following conditions:

- Rotary tube furnace with L/D ratio of 5:1
- Ramp rate of 10°C/min
- 1 hour dwell time
- Thermal efficiency of 80%
- Heat capacity of C = 0.71 J/gK
- Mole ratio of C:SiO<sub>2</sub> = 1:1
- Tap density of C:SiO<sub>2</sub> mixture = 1000 kg/m<sup>3</sup>
- Mole ratio of Mg:SiO<sub>2</sub> mixture = 2:1
- Tap density of Mg:SiO<sub>2</sub> mixture = 1000 kg/m<sup>3</sup>

Electrolysis was calculated as follows:



**Figure S2:** Schematic showing the steps of recycling MgCl<sub>2</sub> into Mg.

**Table S2:** Physical process occurring in each step described in Figure S2, and associated energy requirements

Step	Process	Energy requirement (kWh/kg Si)
A	Sensible heating	1.02
B	Enthalpy of fusion	0.85
C	Electrolysis	69.3*

\*This value was calculated assuming an energy efficiency of 20% for the electrolysis process.

**Table S3.** Data for Figure 4A regarding reaction time and temperatures in 50 literature sources.

Reaction Temp (°C)	Reaction time (h)	Year	Author	doi
800	6	2024	Andriayani <i>et al.</i>	10.1016/j.mset.2023.09.003
800	3	2015	Andriayani <i>et al.</i>	10.14716/ijtech.v6i7.1493
750	2			
850	3			
800	3			
950	3			
700	1.5	2021	Hamedani <i>et al.</i>	10.1002/celc.202100683
700	0			
700	3			
700	6			
650	3	2017	Arunmetha <i>et al.</i>	10.1007/s11664-017-5794-0
600	1	1982	Banerjee <i>et al.</i>	10.1016/0025-5416(82)90046-5
750	1			
850	1			
650	2.5	2007	Bao <i>et al.</i>	10.1038/nature05570
650	2			
650	3	2023	Klinbumrung <i>et al.</i>	10.1007/s12633-023-02380-z
800	0.5	2022	Guo <i>et al.</i>	10.1021/acssuschemeng.2c00632
680	3	2023	Jaswal <i>et al.</i>	10.1016/j.jenvman.2022.116912
650	6	2023	Wang <i>et al.</i>	10.1016/j.electacta.2023.141950
680	3	2023	Su <i>et al.</i>	10.1016/j.cej.2022.138394
750	2	2024	Ma <i>et al.</i>	10.1016/j.cej.2024.148542
700	5	2023	Ma <i>et al.</i>	10.3390/ molecules28073274
660	5			
650	6	2021	Entwistle <i>et al.</i>	10.1039/d0ra09000j
600	1	1982	Banerjee <i>et al.</i>	10.1016/0025-5416(82)90046-5
750	1			
850	1			
700	3	2014	Zhang <i>et al.</i>	10.1002/adma.201402813
675	0.5	2014	Yoo <i>et al.</i>	10.1002/aenm.201400622
900	4	2002	Sandhage <i>et al.</i>	10.1002/1521-4095(20020318)14:6<429::AID-ADMA429>3.0.CO;2-C
600	5	2017	Jiang <i>et al.</i>	10.1016/j.cej.2017.08.061
650	5	2019	Xing <i>et al.</i>	10.1007/s42452-019-0196-y
700	6	2016	Li <i>et al.</i>	10.1038/s41598-017-01086-8
700	1	2014	Chen <i>et al.</i>	10.1007/s12274-013-0374-y
700	2			
700	3			
700	4			

700	5			
680	3	2021	Wang <i>et al.</i>	10.1016/j.jallcom.2020.157955
700	6	2016	Zhou <i>et al.</i>	10.1016/j.jpowsour.2016.05.058
650	7	2013	Xing <i>et al.</i>	10.1039/c3ra41889h
750	3	2016	Xu <i>et al.</i>	10.1039/c6ta01344a
800	12	2014	Xie <i>et al.</i>	10.1039/c4nj00752b
500	7	2015	Shuhe <i>et al.</i>	10.1007/s11595-016-1476-7
800	2	2016	Gao <i>et al.</i>	10.1016/j.electacta.2017.01.119
700	6	2014	Favors <i>et al.</i>	10.1038/srep05623
650	7	2011	Jia <i>et al.</i>	10.1002/aenm.201100485
650	6	2015	Liu <i>et al.</i>	10.1002/ange.201503150
500	1	2013	Xing <i>et al.</i>	10.1039/c3cc43134g
500	12			
700	6	2015	Wang <i>et al.</i>	10.1038/srep08781
700	16	2022	Zuo <i>et al.</i>	10.3390/molecules27217486
800	16			
900	16			
800	5	2019	Falk <i>et al.</i>	10.1016/j.ceramint.2019.07.157
675	2	2012	Yoo <i>et al.</i>	10.1002/adma.201201601
700	1	2026	Waitzinger <i>et al.</i>	10.1007/s00706-015-1611-8
750	1			
600	1	2012	Batchelor <i>et al.</i>	10.1007/s12633-012-9129-8
600	12	2015	Liu <i>et al.</i>	10.1016/j.jmmm.2015.06.074
700	12			
800	12			
800	10	2020	Guo <i>et al.</i>	10.1007/s12613-019-1900-z
800	6			
800	2			
800	14			
700	4	2023	Seroka <i>et al.</i>	10.3390/coatings13020221
650	6	2018	Khanna <i>et al.</i>	10.1139/cjc-2018-0165
650	4	2019	Miao <i>et al.</i>	10.1007/s11581-019-03256-2
650	2	2016	Uehira <i>et al.</i>	10.1246/cl.160544
700	2	2021	Sekar <i>et al.</i>	10.3390/nano11030613
650	3	2018	Tang <i>et al.</i>	10.1016/j.clay.2018.07.004
700	6	2021	Hamedani <i>et al.</i>	10.1002/celc.202100683
700	3			
700	1.5			
700	0			
650	2.5	2011	Chen <i>et al.</i>	10.1149/1.3611433
600	3			
500	3.5			
800	10	2019	Sun <i>et al.</i>	10.1016/j.ijhydene.2019.01.270

## References

1. M. Yan, S. Martell, M. Dasog, S. Brown and S. V. Patwardhan, *Journal of Power Sources*, 2023, **588**, 233720.