HELMHOLTZ ZENTRUM
DRESDEN ROSSENDORF

Yamdb/Goma - “easy” access to thermophysical properties of liquid metals and molten salts

Tom Weier, William Nash, Paolo Personnettaz, Norbert Weber

January 25, 2024

Who am I and what am I talking about?

- Institute of Fluid Mechanics / Department of Magnetohydrodynamics / Liquid Metal Batteries (LMBs)
- chemical engineer by training (Merseburg/Halle-Wittenberg)
- **recreational programmer**
- experimenting on/simulating of LMBs requires knowledge of material properties
- many combinations of liquid metals and molten salts possible ➔ substantial amount of data needed
- extracting data from literature takes time and effort
- treat them as a valuable resource

HZDR
HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

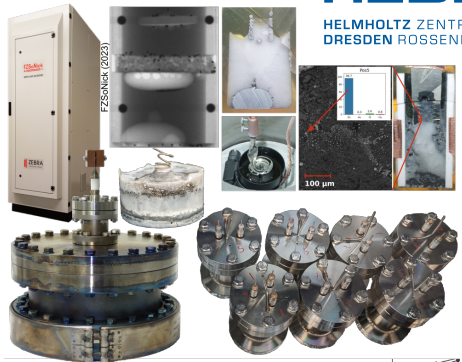


Table 2
Analytical expressions of ionic conductivity of electrolytes measured in this work

Electrolyte	Composition (mol%)	Ionic conductivity (S cm^{-1})
LiCl–LiI	36.4–65.4	13.0462 exp(−907.3/T (K))
LiI–KI	63.3–36.7	10.0001 exp(−1387.9/T (K))
LiCl–LiI–KI	8.5–59–32 • 5	11.0055 exp(−1329.4/T (K))
LiF–LiCl–LiI	11.7–29.1–59.2	8.895 exp(−872.6/T (K))
LiBr–LiCl–LiI	19–24.3–56.7	12.6746 exp(−925.0/T (K))
LiCl–KCl	58.8–42.1	18.7876 exp(−1800.6/T (K))
LiF–LiCl–LiBr	22–31–47	17.8664 exp(−1284.24/T (K))
LiF–LiBr–KBr	0.67–53.5–45.83	20.5817 exp(−1944.76/T (K))
LiCl–LiBr–KBr	12–36.6–51.4	14.1221 exp(−1884.66/T (K))

34.6 [27] no T_m no T_m mass%! Tab 1 : 58.8–41.2

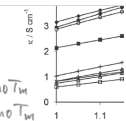


Fig. 6. Evolution of the io
T/T_m) of all electrolytes i
LiCl–LiI, (◯) LiCl–LiBr–
KBr, (▲) LiCl–LiI–KI, (×

What is my Framework?

- goals:
  - small project, minimal dependencies
  - easy data capture
  - portability
  - suitability for REPL (IPython)
  - ➜ dynamic class generation (allowing for tab completion)
  - easy to extend (materials, equations, properties)
- means:
  - YAML for coefficients
  - BibTeX for references
  - SI units only
  - prefer implementation of equations over (error-prone) conversion
  - unit and integration tests with Pytest
  - programming extensions documented in detail

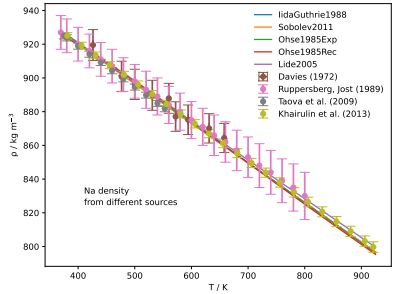
HZDR
HELMHOLTZ ZENTRUM
DRESDEN ROSSENDORF

```yaml
Na:
  Tm: &Tm_Na 370.87
  Tb: 1156.15
  M: 22.98977E-03
  density:
    IidaGuthrie1988: &density_Na_IidaGuthrie1988
      rho_m: 927
      lambda: .235
      equation: Steinberg1974
    Ohse1985:  # recommended  equation
      a:
        - 0.89660679
        - 0.51613430
      default: true
      equation: Shpilrain1985
  dynamic_viscosity:
    Hirai1992:
      A: 0.0846
      B: 6.412
      default: true
      equation: Hirai1992
      comment: "p. 401/63 Tab. 1"
  expansion_coefficient:
    IidaGuthrie1988:
      <<: *density_Na_IidaGuthrie1988
      default: true
```

What are my Challenges and Alternatives?

HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

- interface design, licenses
- Python (Yamdb):
  - \+ pragmatic choice: lingua franca of scientific computing
  - ± dependencies
  - ± NumPy docstrings are sometimes excessive
  - – the Sphinx loves to pose riddles
  - – rapid deprecation
  - – history of package building
- Go (Goma):
  - authors: proven track record
  - simplicity as goal
  - cross-compilation, fast
  - single binaries (no dynamic libraries)
  - > go mod vendor ➔ dependencies in source tree
  - //go:embed ➔ ∼6 MB file contains everything
  - Elisp wrapper ➔ dynamic completion in Emacs
  - promise: Go 2 is never going to happen



Thermophysical properties of Li

property	Temp K	source	value	unit
density	800	Ohse (1985)	483.21	kg/m³
dynamic viscosity	800	Hirai (1992)	0.00031787	Pa · s
dynamic viscosity	800	Ohse (1985)	0.00031594	Pa · s
expansion coefficient	800	Takamichi Iida and Guthrie (1988)	0.0002069	1/K
heat capacity	800	Ohse (1985)	4199.8	J/(kg · K)
resistivity	800	Zinkle (1998)	3.9302e-07	Ω · m
sound velocity	800	Blairs (2007)	4326.9	m/s
surface tension	800	Keene (1993)	0.34787	N/m
thermal conductivity	800	Takachimi Iida and Guthrie (2015)	56.301	W/(m · K)

References

Blairs, S. 2007. "Review of Data for Velocity of Sound in Pure Liquid Metals and Metalloids." *International Materials Reviews* 52 (6): 321–44.