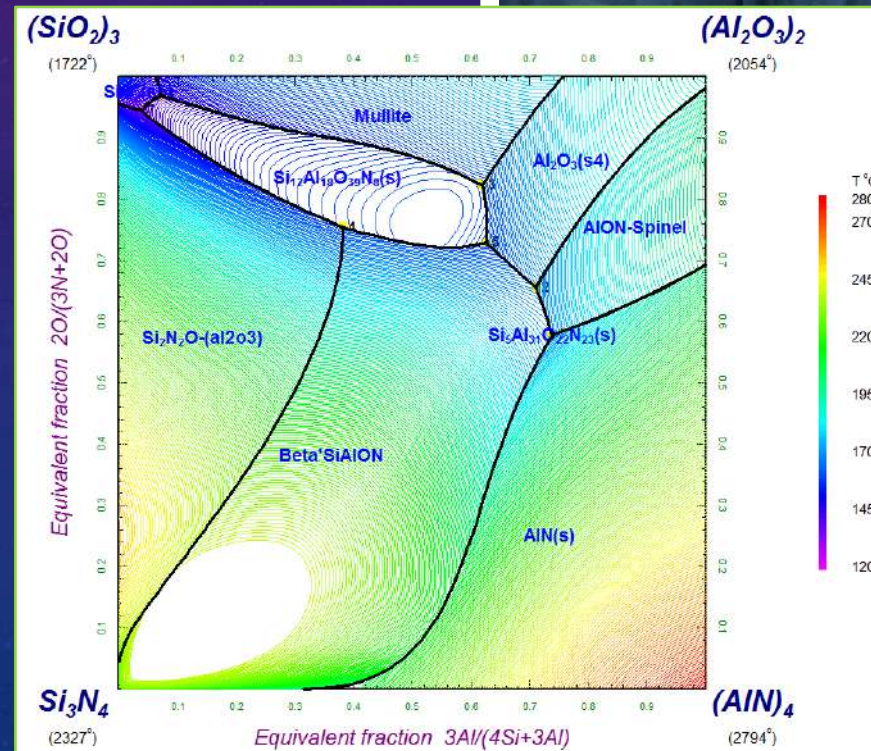# THE PEOPLE OF FACTSAGE

THE SECRET OF SUCCESS IS GETTING TOGETHER A TEAM OF THE BEST PEOPLE AND GETTING THEM TO DO THE WORK

SERGEI DECTER
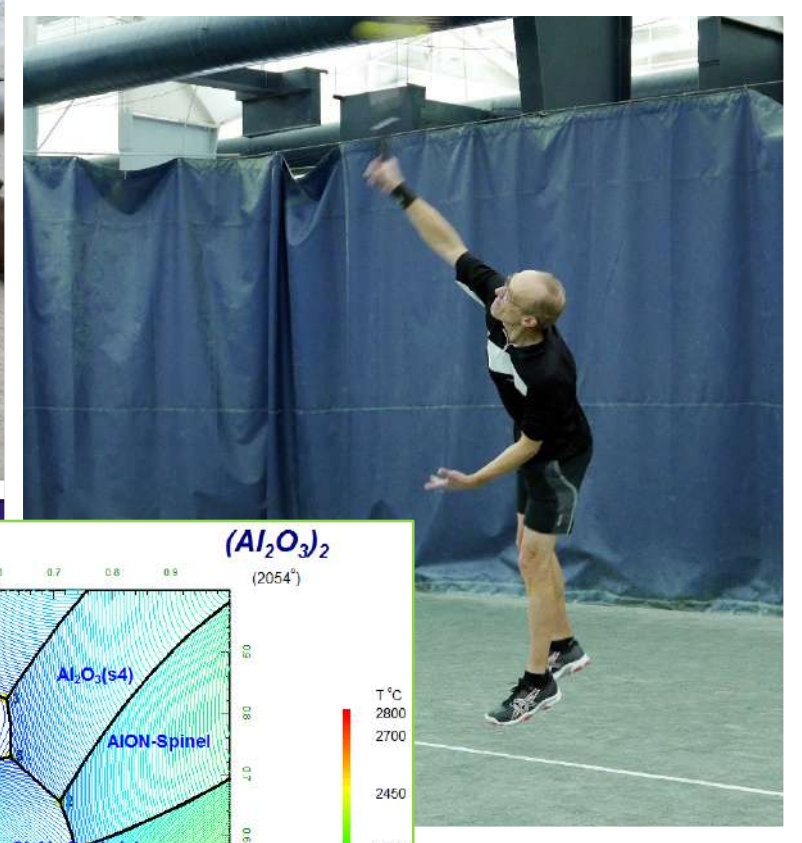
- FToxid (oxide database)

- Viscosity module (oxide melts and glasses)

- Sulfides in database (matte and solid sulfides)

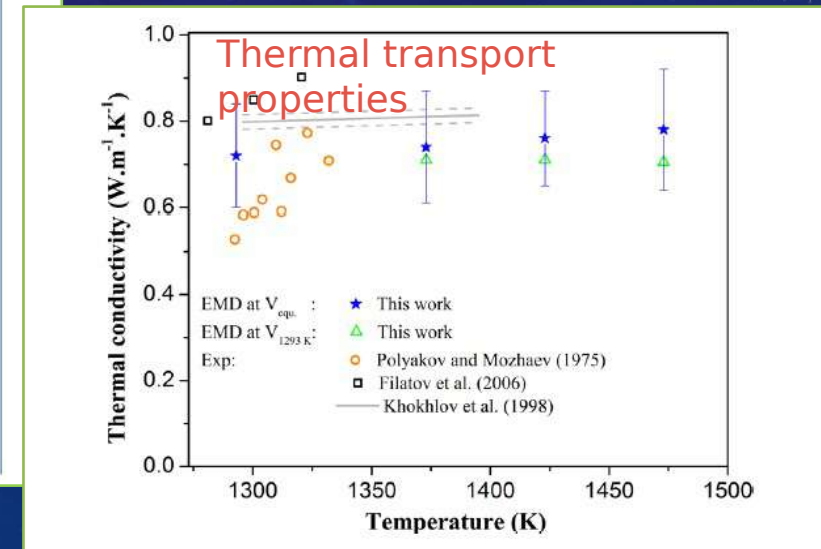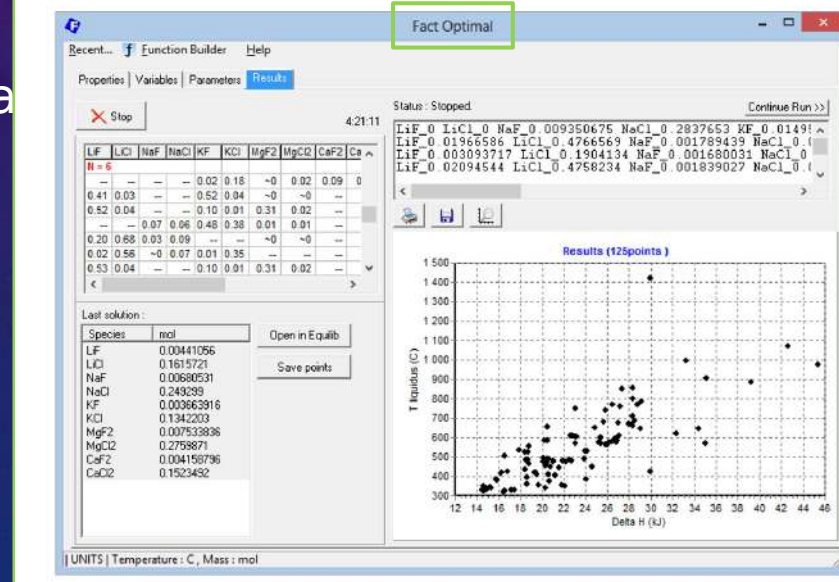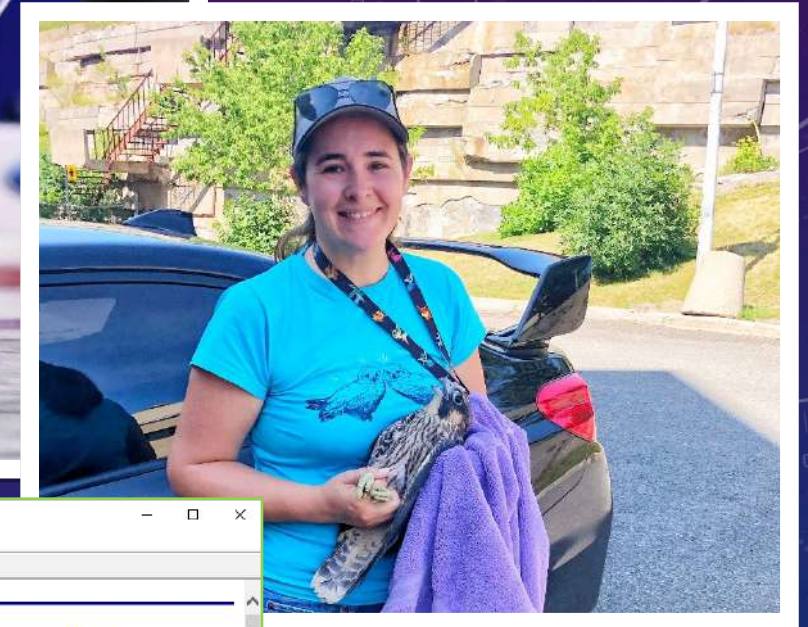- FTOxCN (oxycarbonitride database)

AÏMEN GHERIBI

- FactOptimal software

- Physical properties databa...

- Microstructure module

- Our resident physicist

Calculated *Characteristic Points* in the Li⁺, Na⁺, K⁺, Mg⁺⁺, Ca⁺⁺ / F⁻, Cl⁻ reciprocal system.

Thermal transport properties

EVE BÉLISLE

- FactSage Browser
- FactXML
- Installation software
- Software troubleshooting
- Programming

PATRICE CHARTRAND

- All aspects of FactSage (modelling, programming (Figure), databases)

- Graduate student supervision

- OptiSage optimisation program

- Physical properties

- (Databases: light metals, nuclear, salt, copper, lead, hall, fertilizers, pulp)
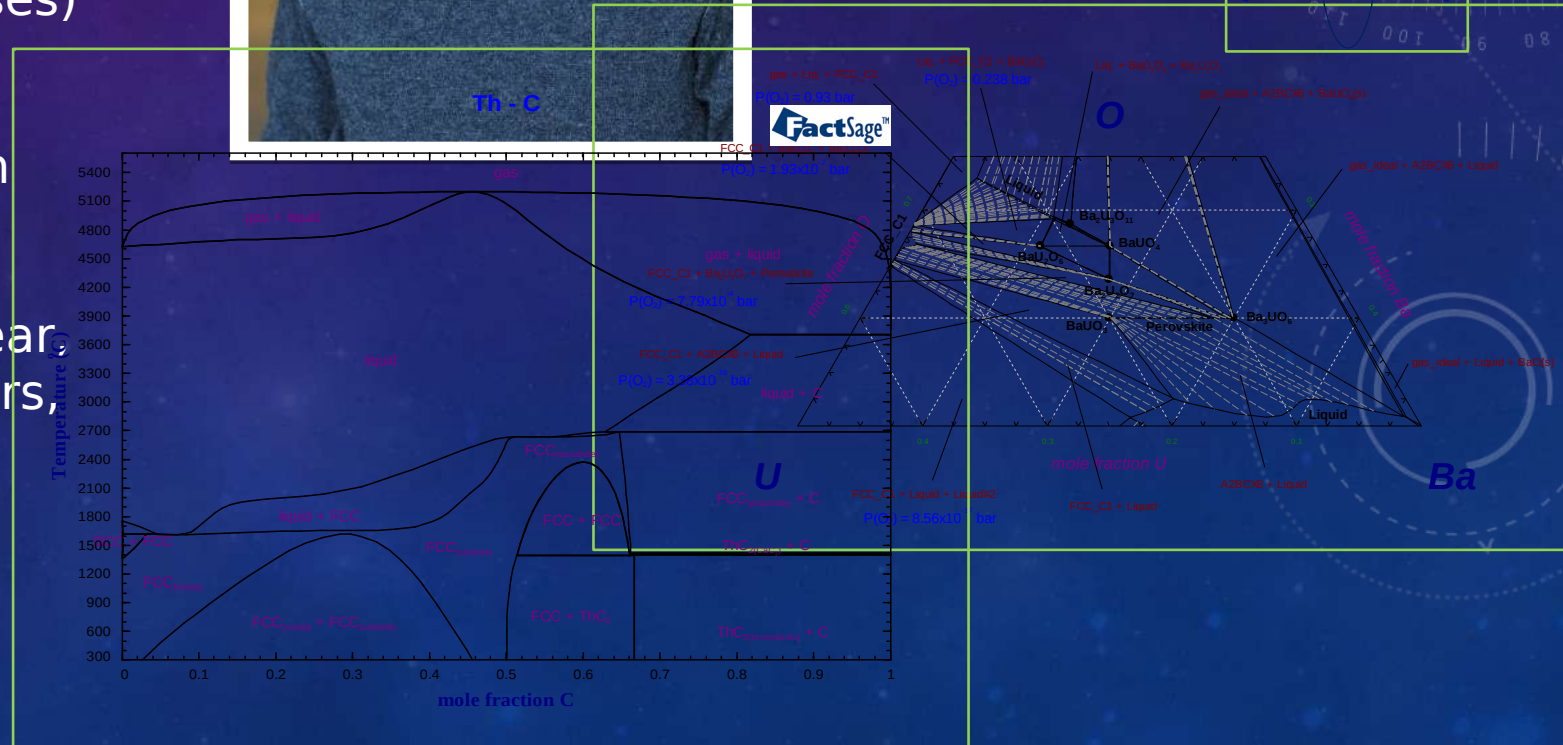
GUNNAR ERIKSSON

- The SOLGASMIX-based Advanced Gibbs Energy minimizer, the heart of FactSage

- OptiSage optimisation program

- Equilib and Phase Diagram program

- ChemApp

Au - Bi - Sb - Pb
Scheil (cooling step 5 K), Pb/(Au+Bi+Sb+Pb)(mol/mol)=0.05, 300 K, 1 bar

Bi

Au   Sb

mole fraction

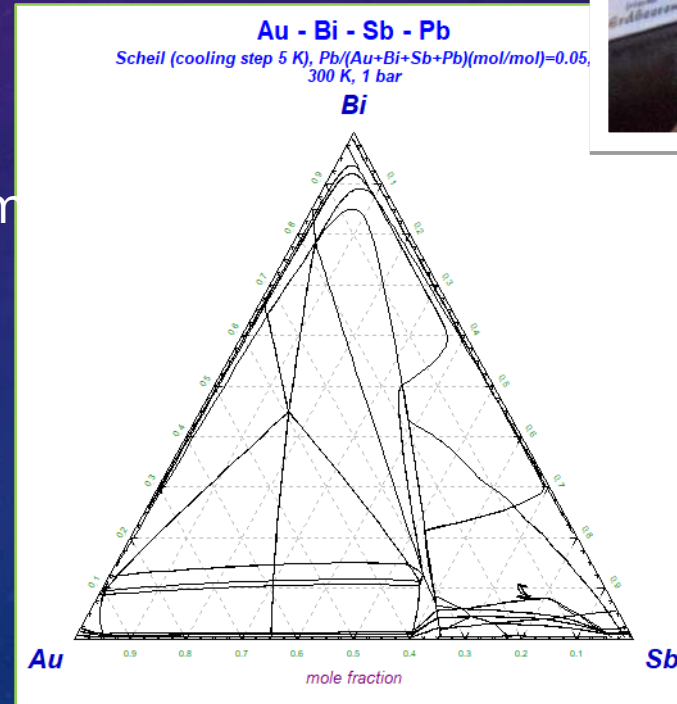| F :	5+8+10	: HCP_A3 + AUSB2 + AuPb2_AUPB2(s)
G :	5+8+9	: HCP_A3 + AUSB2 + Au2Pb_AU2PB(s)
H :	5+6+8+9	: HCP_A3 + RHOMBOHEDRAL_A7 + AUSB2 + Au2Pb_AU2
J :	6+8+9	: RHOMBOHEDRAL_A7 + AUSB2 + Au2Pb_AU2PB(s)
K :	7+9	: AU2BI_C15 + Au2Pb_AU2PB(s)
M :	7+8+9	: AU2BI_C15 + AUSB2 + Au2Pb_AU2PB(s)
N :	7	: AU2BI_C15
P :	7+8	: AU2BI_C15 + AUSB2
Q :	6+7+8	: RHOMBOHEDRAL_A7 + AU2BI_C15 + AUSB2
R :	6+7	: RHOMBOHEDRAL_A7 + AU2BI_C15
S :	6+9	: RHOMBOHEDRAL_A7 + Au2Pb_AU2PB(s)
T :	5+6+9	: HCP_A3 + RHOMBOHEDRAL_A7 + Au2Pb_AU2PB(s)
U :	6	: RHOMBOHEDRAL_A7
V :	5+6	: HCP_A3 + RHOMBOHEDRAL_A7
W :	5+6+8	: HCP_A3 + RHOMBOHEDRAL_A7 + AUSB2
X :	6+8	: RHOMBOHEDRAL_A7 + AUSB2
Y :	3+6+8	: FCC_A1 + RHOMBOHEDRAL_A7 + AUSB2
Z :	3+6	: FCC_A1 + RHOMBOHEDRAL_A7
A2 :	3+8	: FCC_A1 + AUSB2
B2 :	5+8	: HCP_A3 + AUSB2
C2 :	8	: AUSB2
D2 :	3+8+11	: FCC_A1 + AUSB2 + AuPb3_AUPB3(s)
E2 :	8+11	: AUSB2 + AuPb3_AUPB3(s)
F2 :	8+10+11	: AUSB2 + AuPb2_AUPB2(s) + AuPb3_AUPB3(s)
G2 :	6+7+8+9	: RHOMBOHEDRAL_A7 + AU2BI_C15 + AUSB2 + Au2Pb_AU2
H2 :	8+9+10	: AUSB2 + Au2Pb_AU2PB(s) + AuPb2_AUPB2(s)
J2 :	5+8+9+10	: HCP_A3 + AUSB2 + Au2Pb_AU2PB(s) + AuPb2_AUPB
K2 :	3+5+8+10	: FCC_A1 + HCP_A3 + AUSB2 + AuPb2_AUPB2(s)
M2 :	3+7+8	: FCC_A1 + AU2BI_C15 + AUSB2

KLAUS HACK AND STEPHAN PETERSEN

- Database development

- Ideas for new calculational capabilities

- ChemApp

- SimuSage
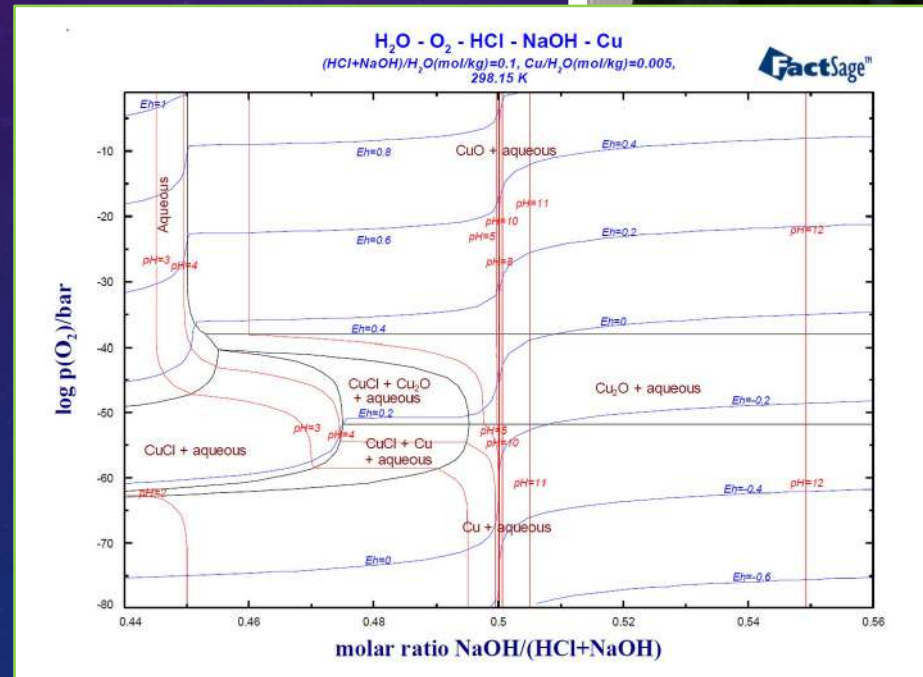
MORITZ TO BABEN, WAJAHAT M. KHAN AND FLORIAN TANG

- Classical and non-classical applications
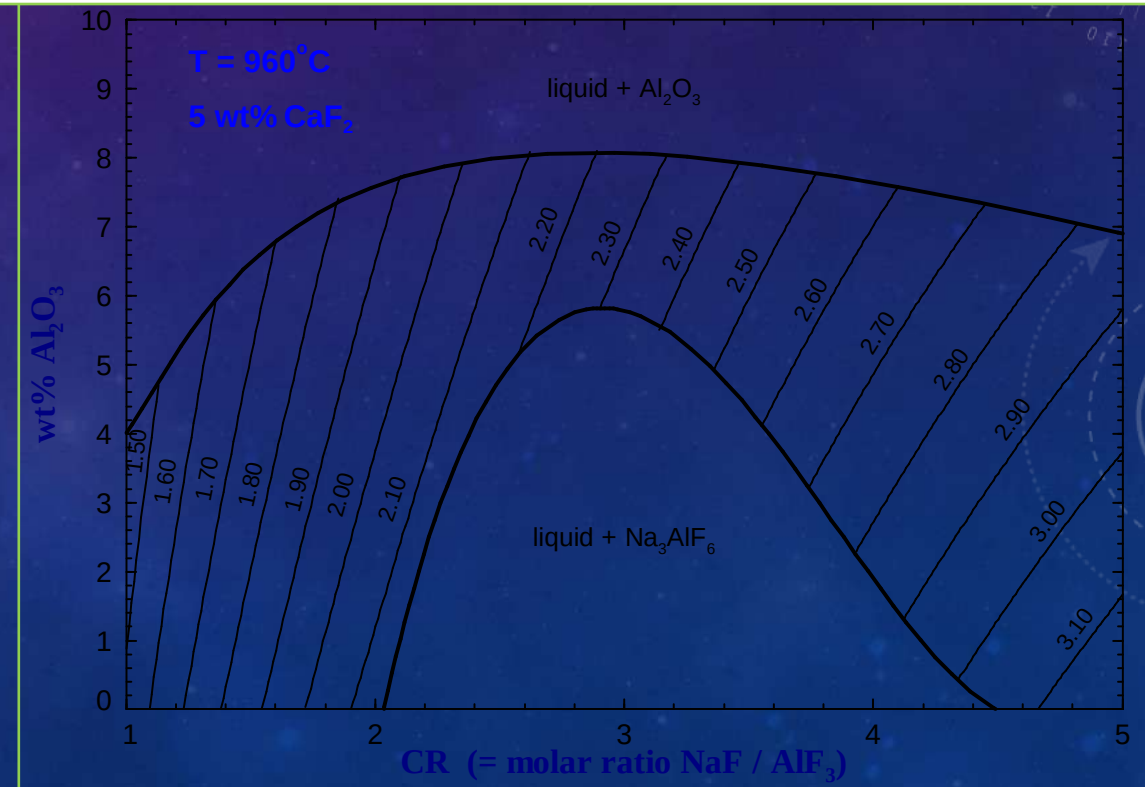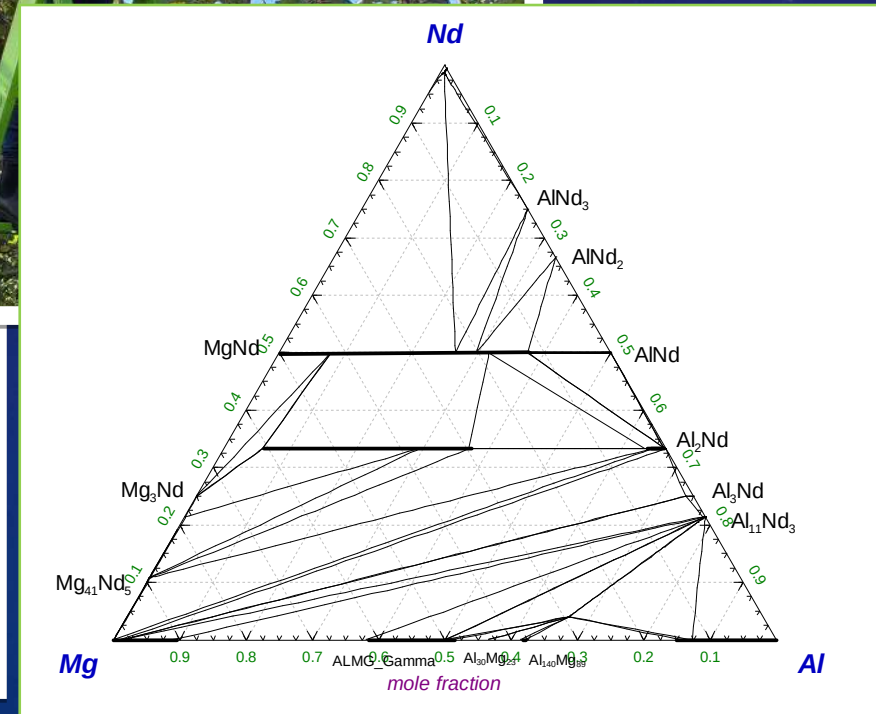- Support
- Security
- TDB converter
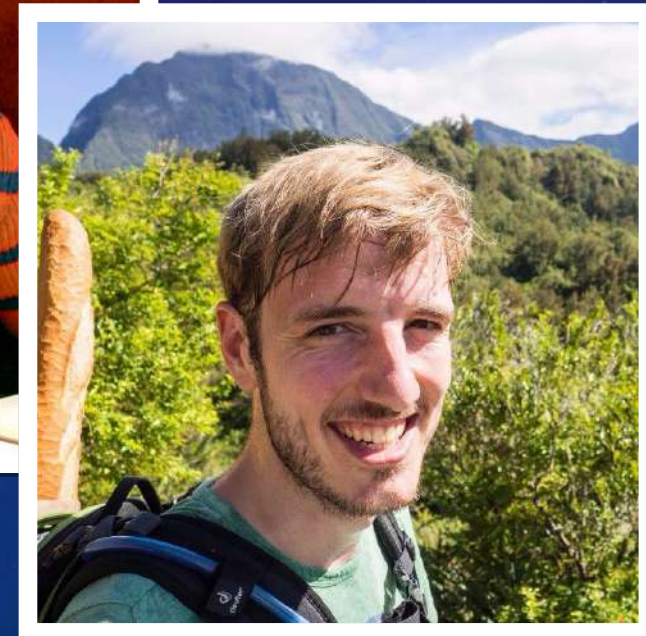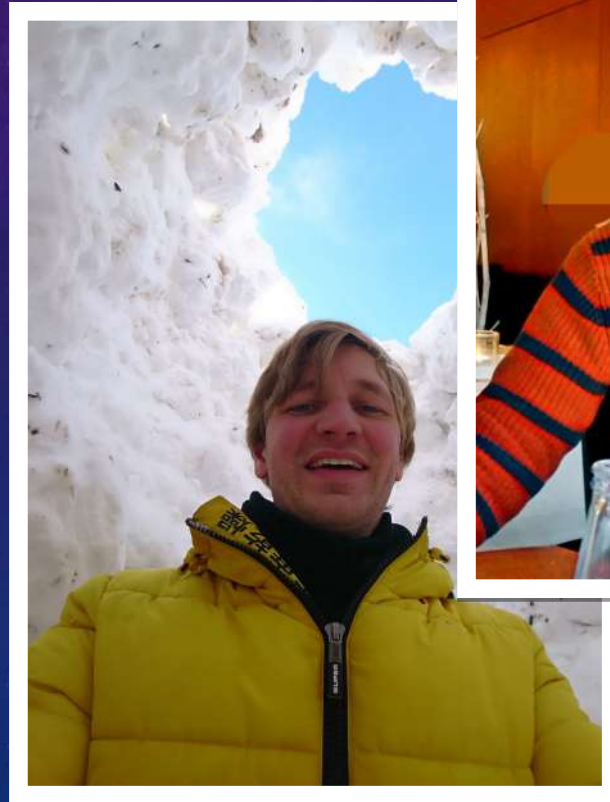
CHRISTIAN ROBELIN

- Development of thermodynamic and physical property databases for inorganic salt systems (FTsalt, FThall, FTfrtz) and ionic liquid systems

Calculated iso-ionic conductivity (S/cm) curves for NaF-AlF_3-CaF_2-Al_2O_3 melts
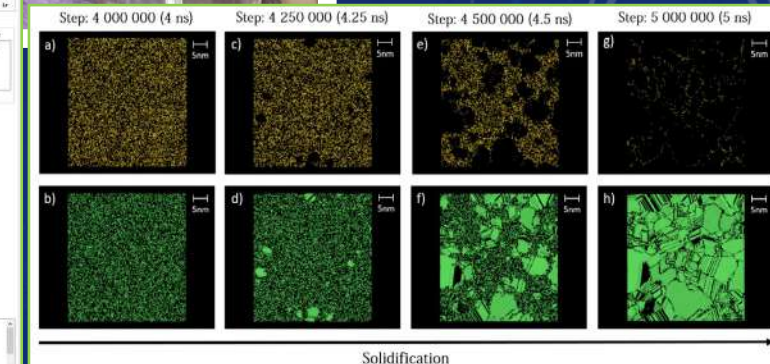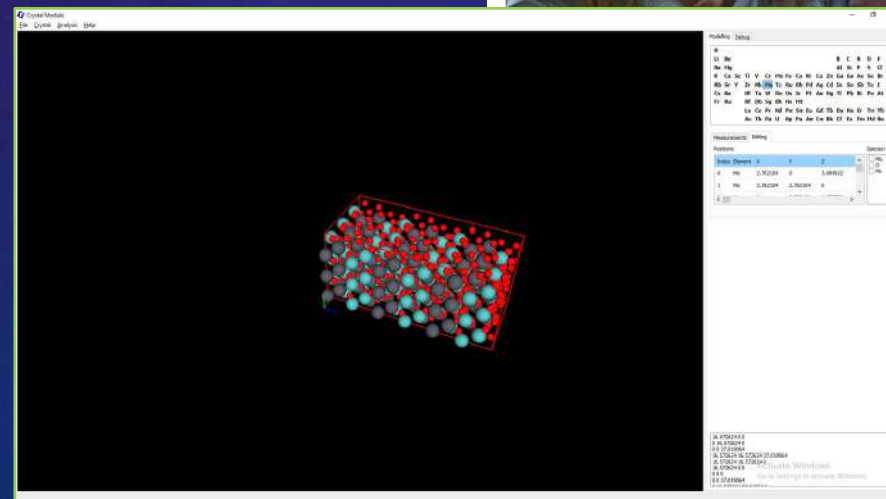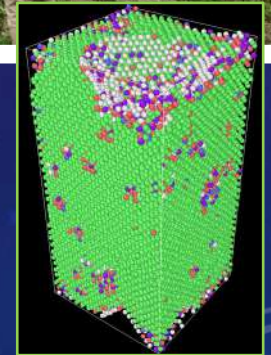
LILING JIN

- Alloy databases development

Ternary phase diagram: Nd – Mg – Al system, mole fraction
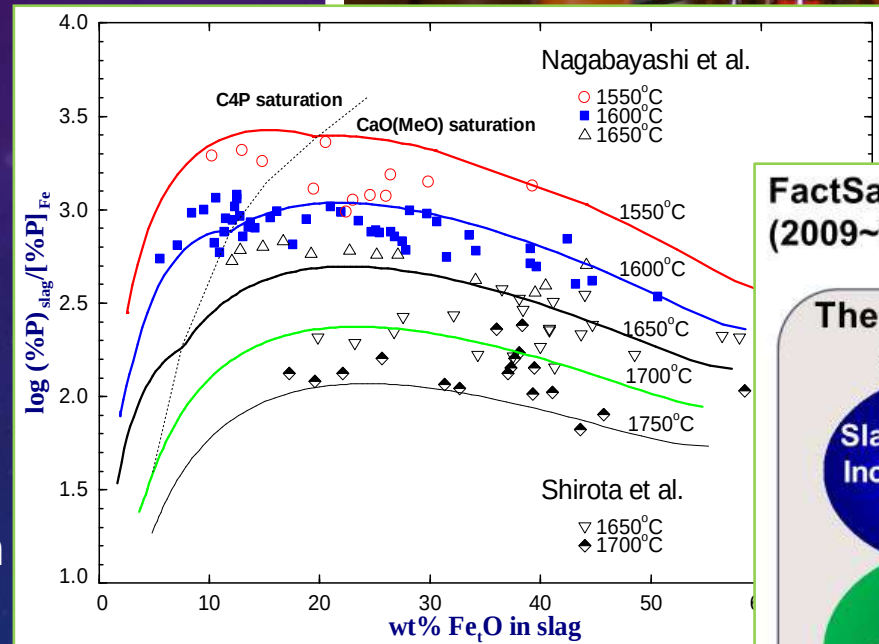
JEAN-PHILIPPE HARVEY

- All aspects of FactSage (modelling, programming, databases)

- Graduate student supervision

- Atomistic simulations (new Crystal module)

- Process simulation
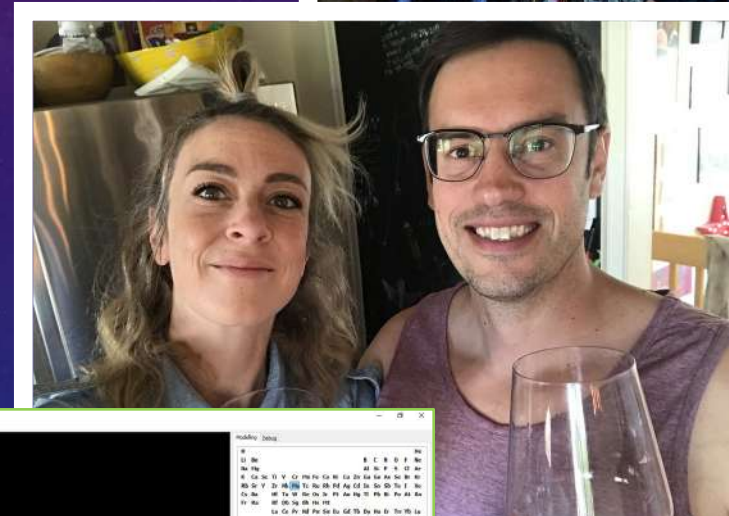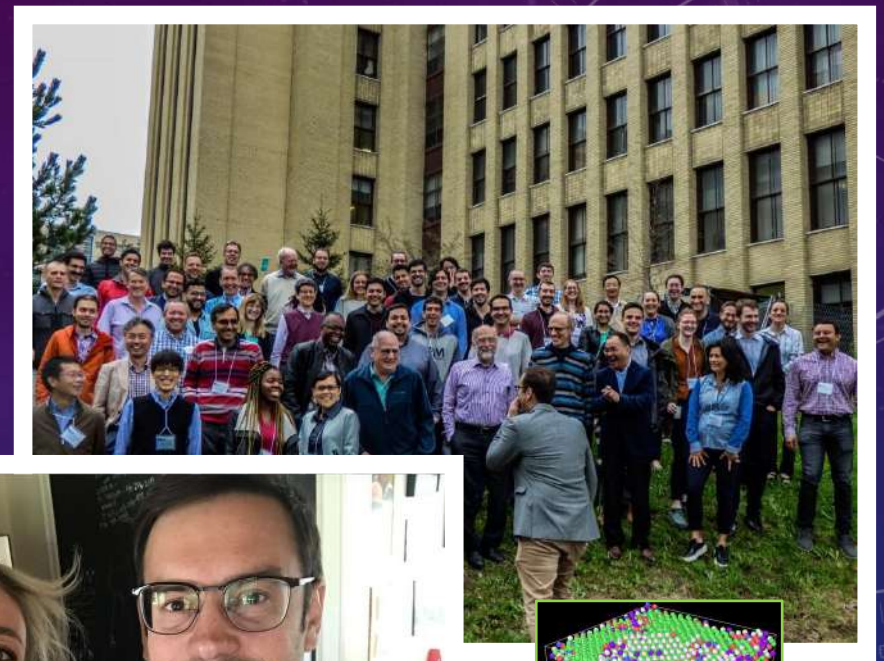
IN-HO JUNG

- FToxid (Oxide) database

- FSstel (Steel) database

- Viscosity database

- Application of FactSage for pyrometallurgical process and alloy design

- Steelmaking Consortium Project (12 companies)

- FIRE Refractory Consortium Project (7 companies)

YOUN-BAE KANG

- Oxide (+ oxysulfide) database/
  alloy database development

- Application to
  steelmaking/casting process

- Model performance validation
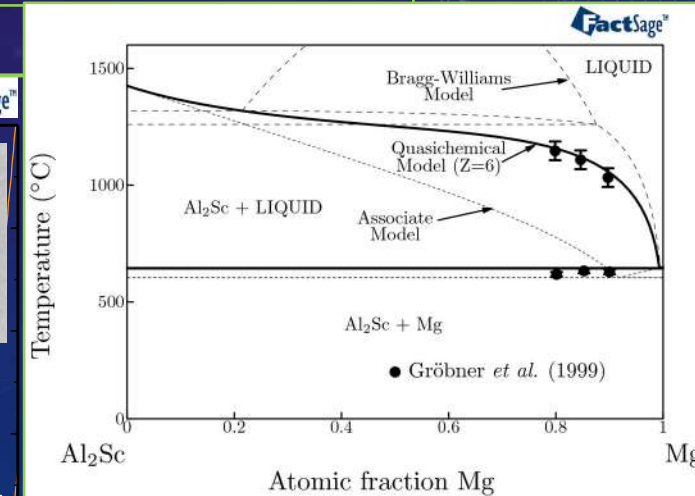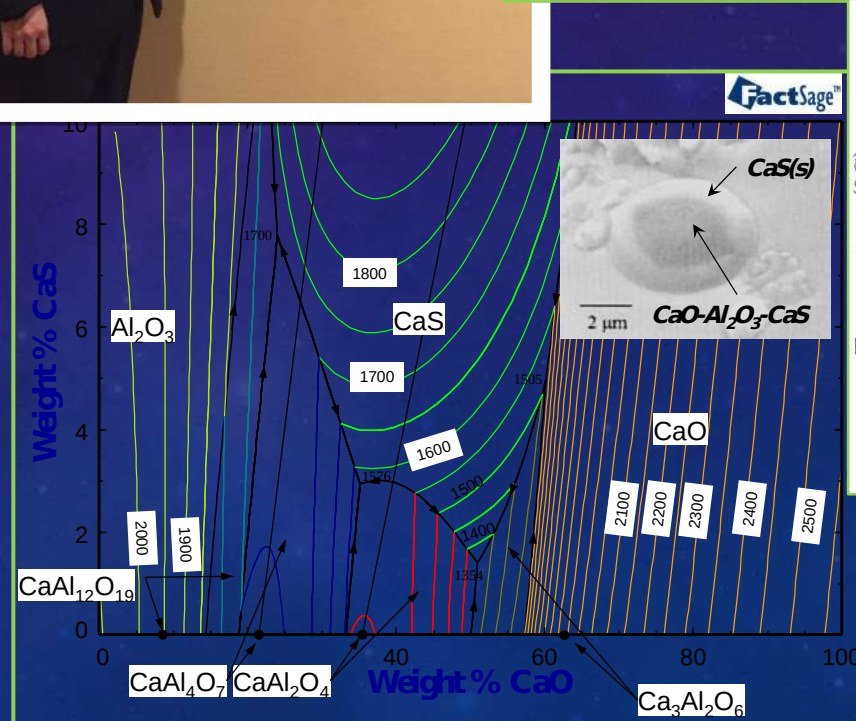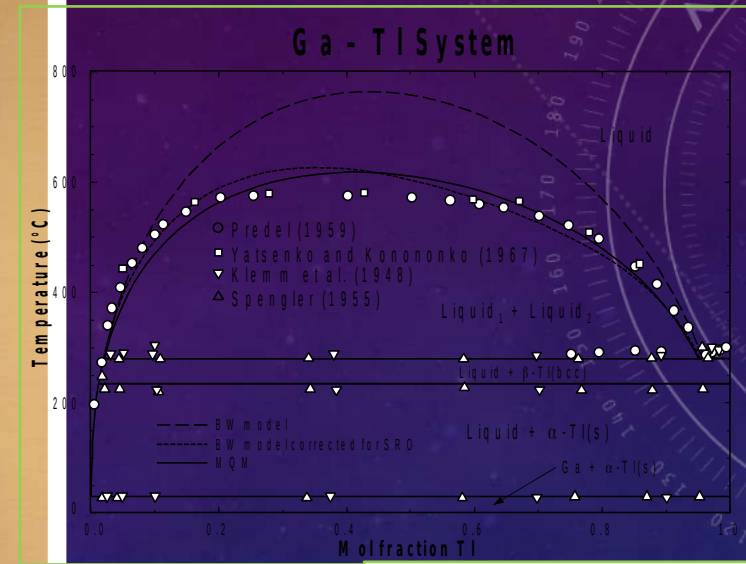
JACQUES MELANÇON

- Compound module
- Solution module

MARIE-ALINE VAN ENDE

- FactSage Macro Processing (workshops and process simulations)

- Applications of FactSage for pyrometallurgical processes
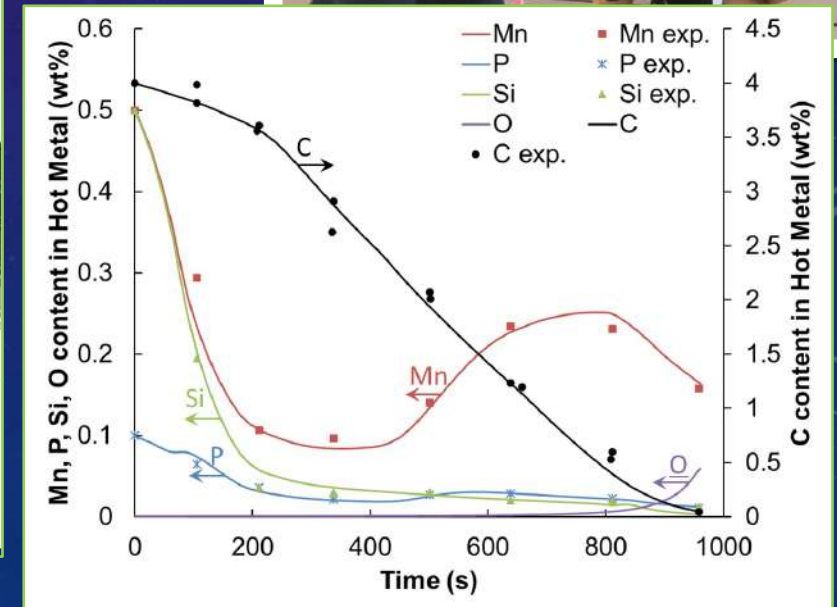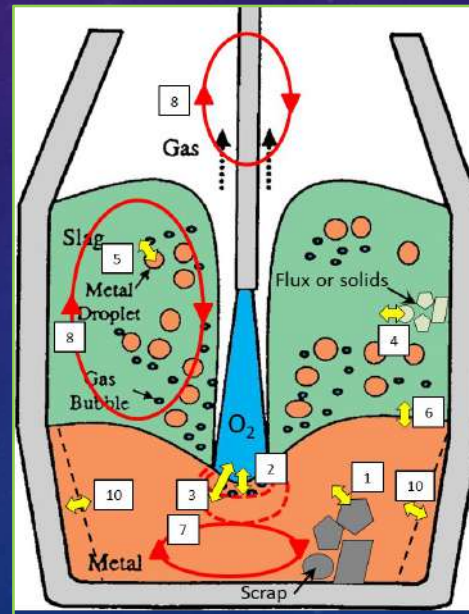
PHILIP SPENCER

- Steel database

- Refractory alloy database

- Noble metals database

- Light metals, copper, lead, ultrapure silicon databases
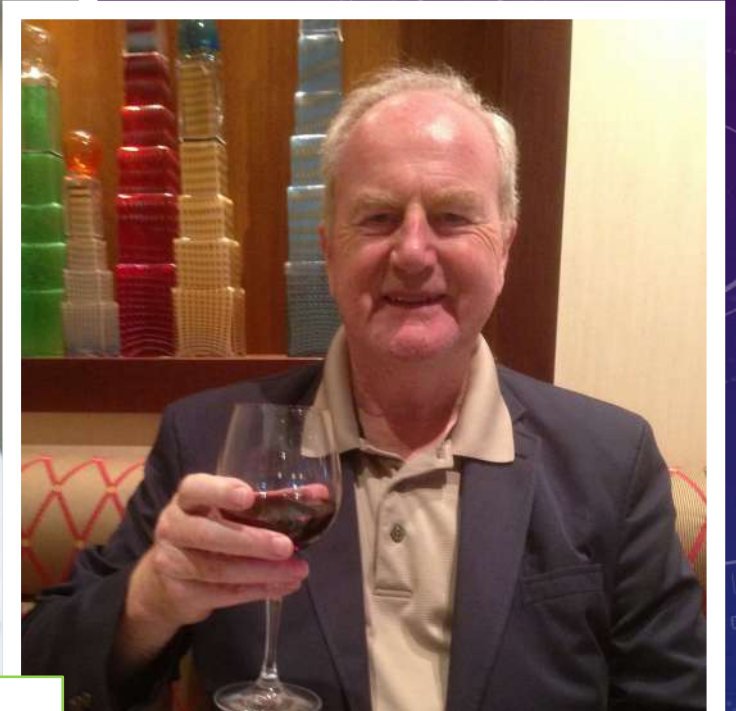
BILL THOMPSON

- A founding father of FactSage

ZHANMIN CAO AND DAIGEN FUKAYAMA

- Beta-testing and error checking
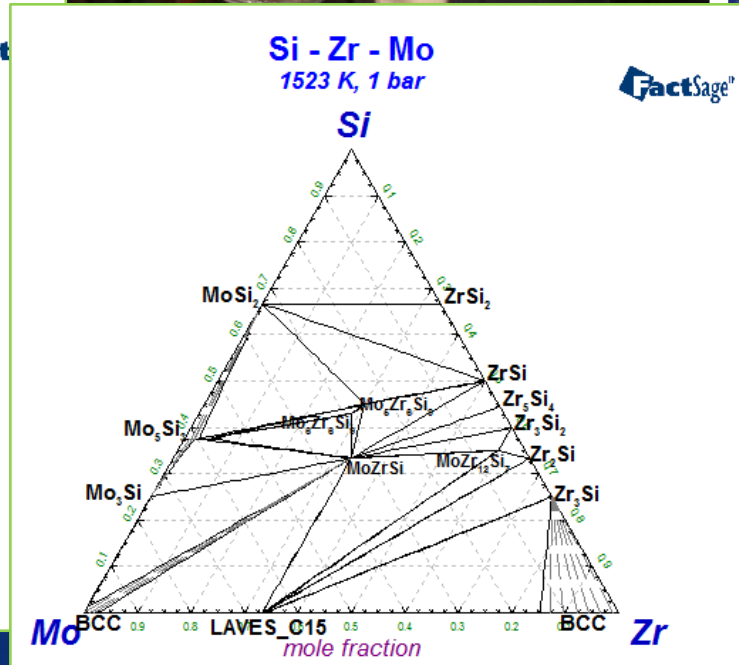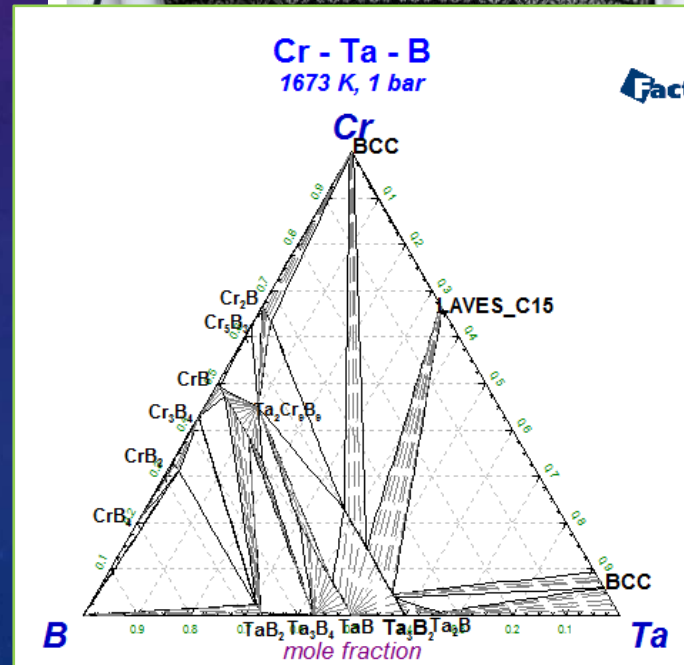
JAMES SANGSTER

- FACT pure substances database

THERMODYNAMIC PROPERTIES OF BINARY SYSTEMS OF DRUGS

FIG. 24. The system 4-nitrophenol (A)+etofylline (B).

EVGUENIA SOKOLEN

- Technical assistance

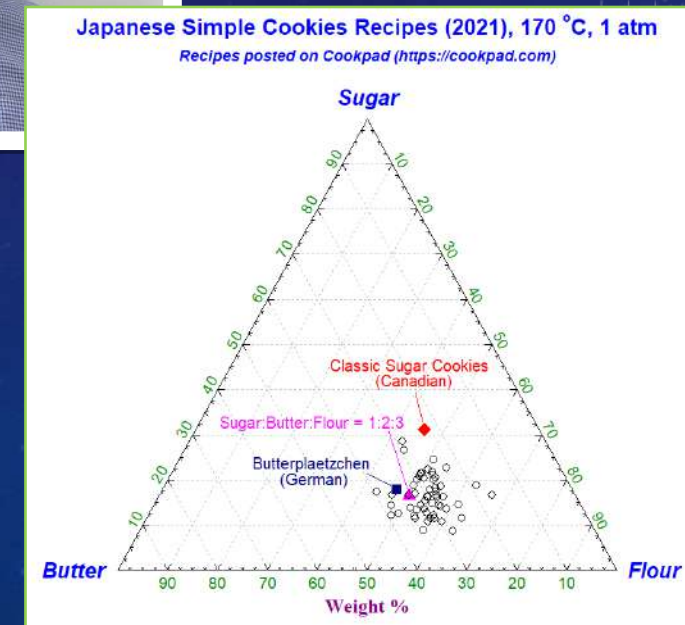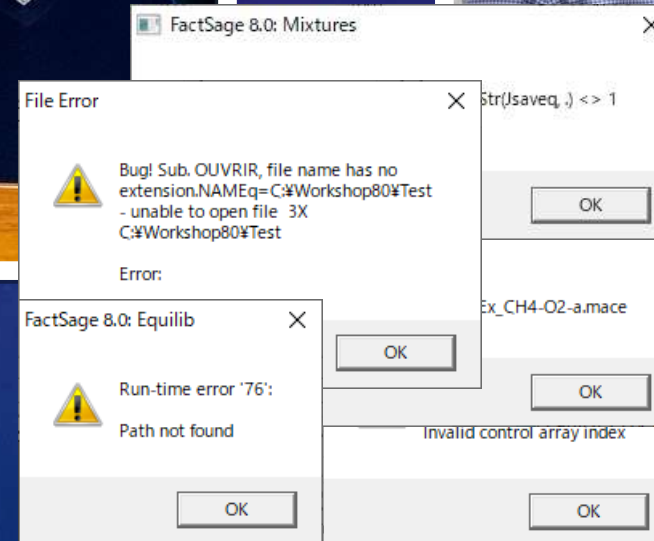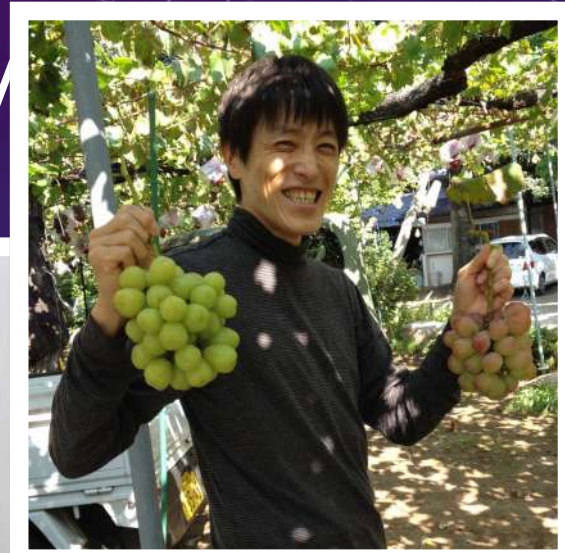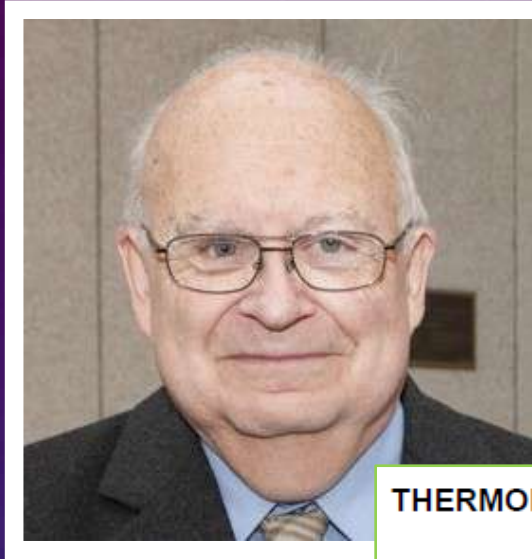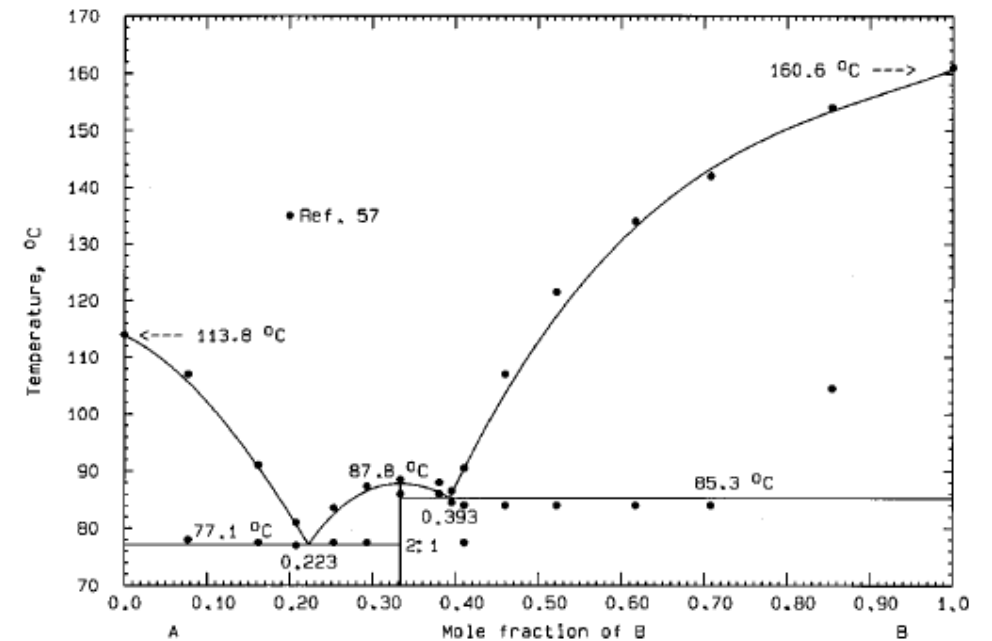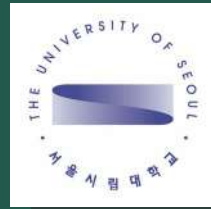# COLLEAGUES AND COLLABORATORS

Polytechnique Montréal, Université d'Ingénierie

- Dr. Patrice Chartrand
- Dr. Jean-Philippe Harvey
- Ms. Eve Bélisle, M.Sc.
- Dr. Sergei Decterov
- Dr. Aïmen Gheribi
- Dr. Jacques Melançon
- Dr. Christian Robelin
- Dr. James Sangster
- Dr. Liling Jin
- Ms. Evguenia Sokolenko

The Spencer Group

- Dr. Philip Spencer

The University of Seoul

- Prof. In-Ho Jung
- Dr. Marie-Aline Van Ende

GTT-TECHNOLOGIES

- Dr. Gunnar Eriksson
- Prof. Klaus Hack
- Dr. Stephan Petersen
- Dr. Juergen Korb
- Dr. Moritz to Baben
- Dr. Wajahat Kahn
- Dr. Florian Tang

FactSage representatives

- Gwen and Philip Spencer   (USA)
- Yuichi Nagano   (Japan)
- Zhanmin Cao   (China)
- In-Ho Jung   (Korea)
- Tridiagonal Ltd.   (India)
- Marinda Zietsman   (S. Africa)
- Eugene Jak   (Australia)
- Peilin Mao   (Singapore)
- Nubia Cardona Valencia   (S. America)
- Leonardo Barboza Trindade   (Brazil)
- Tanai Marin   (N. America)
- Dr. Dennis Shishin   (U. Queensland)
- Dr. Viktoria Prostakova   (U. Queensland)
- Prof. Zhanmin Cao   (USTB)