Advanced Geochemical Modeling from Atomic to Macroscopic Scale
Duration: One day. Half day macroscopic modeling with emphasis on tools and applications. Half day on quantum-mechanical atomistic simulations of thermodynamic properties of minerals by first principles density functional theory (DFT) and statistical mechanics with a glimpse of molecular dynamics (MD).

Course objectives
At the end of the short course, students will be able to:

- Become familiar with the concepts, tools, and range of geochemical modeling applications;
- Understand, with the help of detailed explanation, a few examples of geochemical modeling as a tool to interpret natural and engineered systems; and
- Use popular geochemical modeling software packages such as PHREEQC and ToughReact.
- Understand and use physically-consistent thermodynamic datasets outside the black-box approach

Students will enhance their problem-solving skills and quantitative skills through problem sets and modeling exercises.

Course Overview
Geochemical modeling is a powerful tool, which has wide applications such as geothermal energy, CO_2 storage in saline aquifers and basalts, and groundwater contamination and remediation. Recently, new databases, code enhancements, and utilities associated with computer programs have expanded the applicable ranges of these modeling tools. This short course will introduce these new tools and use examples to demonstrate these expanded geochemical modeling capabilities with examples. Special attention will be devoted to the use of first principles-constrained thermodynamic datasets for geochemical modelling and their application to phase equilibrium calculations up to very high pressure and temperature conditions. Practicals and hands-on tutorial on Gibbs free energy minimization method by in-house computer codes will be also provided during the short course.

Suggested Reading
Parkhurst, D. L., & Appelo, C. A. J. (2013). Description of input and examples for PHREEQC version 3: a computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations (No. 6-A43). US Geological Survey.

Zhu C and Anderson GM (2002) *Environmental Applications of Geochemical Modeling*. Cambridge University Press, London, 304 pp. weblink

Zhu, C. & Nordstrom, D. K. Flying Blind: Geochemical Modeling and Thermodynamic Data Files. *Groundwater* **n/a** (2022). https://doi.org:https://doi.org/10.1111/gwat.13223

Zimmer, K., Zhang, Y., Lu, P., Chen, Y., Zhang, G., Dalkilic, M., & Zhu, C. (2016). SUPCRTBL: a revised and extended thermodynamic dataset and software package of SUPCRT92. Computers & Geosciences, 90, 97-11

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The instructors

Chen Zhu is a Professor at Indiana University, USA. Chen is the co-author of the book with Greg Anderson, *Environmental Applications of Geochemical Modeling* published by Cambridge University Press, which is used as a textbook at universities around the world. Chen has worked on all three aspects of geochemical modeling: fundamental geochemistry underlying modeling, computer codes and databases, and applications to geological carbon sequestration, nuclear waste disposal, diagenesis, and groundwater contamination and remediation. Zhu holds a Ph.D. from Johns Hopkins University, an MSc from the University of Toronto, a BS from the Chengdu University of Technology, and a postdoctoral fellowship at the Woods Hole Oceanographic Institution. Zhu was a Fulbright Scholar and the 2006 recipient of the John Hem Award from the (US) National Ground Water Association. Zhu has been elected a fellow of the American Association for the Advancement of Science, the Mineralogical Society of America, and the Geological Society of America. He was a visiting professor at University of California – Berkeley, ETH, and CNRS among other institutions, and recently awarded a visiting professorship at the University of Cambridge in UK. Recently, served as the 2021-2022 Henry Darcy Distinguished Lecturer sponsored by the (US) Groundwater Foundation and gave 67 lectures around the world.

Donato Belmonte is an Associate Professor at the Department of Earth, Environment and Life Sciences (DISTAV) of the University of Genoa, Italy. His research activity focuses on the following topics: i) thermodynamics and lattice dynamics of Earth and planetary materials (solids, glasses and liquids) at extreme P-T conditions; ii) *ab initio* simulation of thermodynamic and thermoelastic properties of crystalline solids by density functional theory (DFT); iii) phase diagram calculation in complex multi-phase systems by computational thermodynamics; iv) molecular dynamics simulation of melting processes and solid-liquid-gas phase equilibria at planetary conditions. He gained a PhD in computational geochemistry at University of Genoa in 2013, then he was invited visiting professor at the Institut de Physique du Globe de Paris (IPGP) in 2016 and very recently at the Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, Paris in 2025. He is currently elected Council Member and Treasurer of the Italian Society of Mineralogy and Petrology (SIMP) for the period 2022-2026. He gave lectures and invited seminars at several international PhD schools, workshops and meetings.