Abstract:

In this talk, I would like to highlight the importance of classical thermodynamics as a numerical tool in order to improve our fundamental understanding in various fields of earth and planetary sciences, with a particular attention to phenomena involving the presence of silicate melts under high pressure. To do so, I will first revisit some of the important concepts and strategies used to identify the equilibrium state of a given multicomponent system identified by sequentially solving a series of key constrained minimization problems. The selection of the adequate thermodynamic model and its subsequent parameterization procedure to ensure good interpolations/extrapolations abilities will then be discussed. Actual limitations imposed by experiments and their consequences on our ability to parameterize and improve existing models will also be highlighted, as well as the most recent numerical tools available like molecular dynamics and Monte Carlo method used to partially circumvent these problems. Then, I will work out some examples (Sept-Iles layered mafic intrusion, copper deposit origin, blast furnace operation) to demonstrate various types of equilibrium conditions that can be imposed to a system, apart from the simple mass balance constraints, and the window of opportunities these “new” types of calculations can bring. Finally, I would like to expose the importance of classical thermodynamics as a tool to design experiments, validate observations, and predict phenomena under a wide range of equilibrium conditions. This will allow me to identify different bridges of knowledge classical thermodynamics can build between different scientific disciplines.