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### **Abstract Information**

Abstract ID: 23159

#### **Abstract Text:**

Thanks to the bright and responsible computer science undergrads Ranvir, Kevin, and Rob, the geochemical community now has a science gateway for geochemical modeling at https://models.earth.indiana.edu/, (and upcoming: geochemsim.org). About ~7000 users/visitors from 89 countries used these programs in the past two years for teaching and research.

The gateway hosts programs SUPCRTBL [1], Online PHREEQC,  $CO_2$  Solubility Calculator, Reaction Rate Calculator, and  $H_2S$  Solubility Calculator. Notably, the Online PHREEQC program together with our customized databases now allows speciation and solubility and reaction path modeling to temperatures up to 1000 °C and pressure up to 5000 bars [2]. Recently, an internally consistent thermodynamic database for rare earth element crystalline solids with 155 endmembers for phosphates [3], oxides, hydroxides, chlorides, fluorides, carbonates, hydrous carbonates, and ferrite are added to SUPCRTBL and PHREEQC.

The science gateway is hosted on Indiana University's high-performance computers. The format of open-source and science gateway technologies answers the call from the U.S. National Science Foundation's FAIR guiding principles (Findability, Accessibility, Interoperability, and Reuse).

- 1. Zimmer, K., et al., Computers & Geosciences, 2016. **90, Part A**: p. 97-111.
- 2. Zhang, G.R., et al., Computers & Geosciences, 2020. **143**.
- 3. Pan, R., et al., Minerals, 2024. **14**(3): p. 305.



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critical minerals, geochemical modeling and rare earth elements

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### **Preferred Presentation Style:**

Poster

#### **Conference Attendance:**

In person

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