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PyGeoChemCalc as an Open-Source Tool for Automating Thermodynamic Calculations and Data Integration

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With the growing focus on understanding water-rock interactions across terrestrial planets and addressing challenges in diverse geo-environmental systems, the need for robust, accessible, and interoperable geoscience tools has never been greater. In an era where data-driven insights drive advancements in geochemistry, amidst a plethora of scientific and engineering advances, such tools are essential for accelerating research, improving data accessibility, and ensuring reproducibility across a range of scales. PyGeoChemCalc (PyGCC), an open-source Python package [1], is designed to bridge critical gaps in geochemical modeling by providing an integrated suite of functions for calculating the thermodynamic properties of aqueous, mineral, and gas species, including mineral solid solutions and variable-chemistry clay minerals. This presentation will highlight how PyGCC's modularity enhances geochemical workflows by streamlining thermodynamic calculations and enabling seamless integration with geochemical modelling platforms, such as Geochemist's Workbench, PFLOTRAN, and EQ3/6. By leveraging PyGCC's ability to estimate thermodynamic parameters across a broad range of temperature and pressure conditions, researchers can refine speciation, reaction path and reactive transport models, improving predictive capabilities, and accelerating the translation of fundamental geochemistry into practical applications. We will present case studies demonstrating how PyGCC accelerates geochemical insights in various water-rock interactions, emphasizing the need for its broader adoption. As we navigate the transition to a sustainable energy future and strive to address open scientific questions about various terrestrial planets, open-source tools like PyGCC are key to fostering innovation, improving model predictability, and ensuring that geochemistry remains at the forefront of global scientific challenges.

[1] A. N. Awolayo, B. M. Tutolo, PyGeochemCalc: A Python package for geochemical thermodynamic calculations from ambient to deep Earth conditions. *Chem. Geol.* **606**, 120984 (2022).