Molecular level simulations of the H_2O, CO_2 and CO_2-H_2O systems up to high temperatures and pressures

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H_2O, CO_2 and CO_2–H_2O are the most frequently encountered fluid systems in and around the Earth, widely existent in various geospheres, as revealed from direct measurements or from the study of fluid inclusions in various rocks and ore deposits. In this study, we have carried out a series of molecular dynamics and Monte Carlo simulations to predict the properties of these systems up to high temperatures and pressures, which are difficult or even impossible to attain with experimental measurements.

For pure water, we selected a potential model (SPCE) established at normal temperature and pressure and found remarkable reproducibility of molecular dynamics simulations over wide temperature and pressure ranges. Compared with the most recent published high-pressure experimental data up to 5.0 GPa, the simulation results show very good agreement with errors less than 1.0% and reveal a trend to be more accurate as the increase of pressures.

For carbon dioxide, we have proposed an optimized potential model utilizing the established techniques of molecular dynamics and histogram reweighting grand canonical Monte Carlo simulations. This model is demonstrated to show excellent predictability for thermodynamic, transport, and liquid structural properties in a wide temperature-pressure range with remarkable accuracies.

Thereafter, through comprehensive isothermal-isobaric molecular dynamics simulations, the pressure-volume-temperature-component (*PVTx*) data of CO_2-H_2O have been extended beyond experimental range (below 1673.15 K, 1.94 GPa) to about 2573.15 K and 10 GPa.

Finally, an equation of state (EOS) was laboriously developed for the H_2O, CO_2 and CO_2–H_2O systems. This EOS reproduces all the experimental and simulated data covering a wide temperature and pressure range from 673.15 to 2573.15 K and from 0 to 10.0 GPa within experimental or simulation uncertainty.

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Diagenetic environment of Qingbulake basic complex, Xinjiang, NW China

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The Qingbulake basic complex is located 120km southeast to the Tekesi County, Xinjiang, NW China. As the Sm-Nd age is similar to the Karatunk complex in the south margin of Altay orogenic belt and Huangshandong complex in eastern Tianshan, these intrusions were considered to be formed in the similar post-collisional environment.

In this study, the high precise SHRIMP zircon U-Pb age of 434±6.2 Ma for diorite from the complex reveal that the major mafic magmatic events took place in the early to middle Silurian. According to recent research on the regional tectonic evolution (e.g., Li *et al*., 2006, Gao *et al*., 2006), at least in early Silurian, the southern Tianshan oceanic crust began the subduction to central Tianshan plate and ended in early Carboniferous. Geochemical studies of the Qingbulake basic complex show that it is characterized by low content of Ti, depletion of Nb and Ta and enrichment of large lithosphile elements and slight enrichment of LREE. The magma also displays some features of inland arc magma (Zhang *et al*., 2006).

So the Qingbulake mafic complex may be closely related to the subduction of southern Tianshan ocean crust to Yili-Central Tianshan plate.

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