

Silicon Uncommon in Deep Earth

Objective: Investigate structural properties of silica (SiO_2) and other materials under extreme conditions.

Implications: One of the most ubiquitous and important minerals, SiO_2 is used in ceramics, electronics, and glass. But its abundance and role in the structure and dynamics of deep Earth is still unknown.

Accomplishments: Quantum Monte Carlo results suggest that Silica populates Earth only superficially; it's relatively uncommon deep within the Earth.

- Results document improved accuracy and reliability of QMC relative to the more common and efficient Density Functional Theory method; increased role seen.

NERSC: Key pre-production FranklinQC user, 3Mhours; CASINO code; 4-4k cores, avg. 420

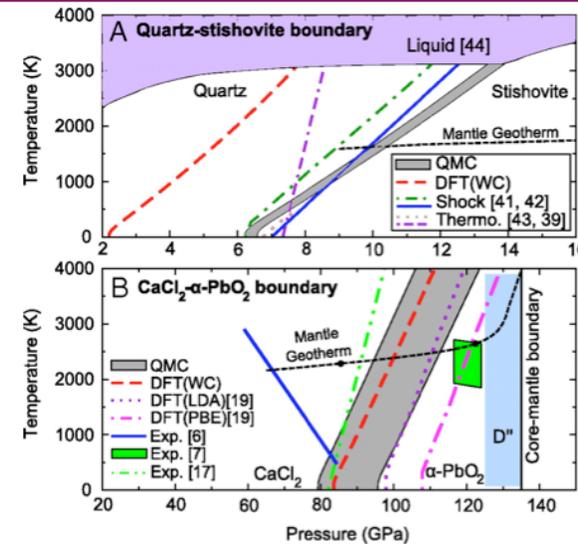


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Computed phase diagrams that reveal at which temperature (vertical) and pressure (horizontal) within the Earth the various forms of silica are stable. Results suggest that there is little or no free silica in the bulk of the lower mantle.

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