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Fate of germanium in Earth's crust

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Germanium (Ge) is a rare but critical element used in semiconductors, light-emitting diodes (LEDs), integrated circuits (ICs), photovoltaic (PV) cells and 5G networks. It is also used as catalyst in the petrochemical industry. Despite its high industrial demand, reliable primary deposits remain unidentified. Currently, germanium is primarily sourced from the recycling of electronic waste and zinc and coal mine by-products. Its crustal concentration (1.5 ppm) is similar to that of tungsten and molybdenum, which are mined as main products. Ge is rare because it is located below silicon (Si) in the periodic table, sharing similar valence-shell configurations and atomic radii, enabling Ge to substitute for Si in silicates, which prevents the formation of its own mineral deposits.

Previous research shows that $Ge(OH)_4$ and $Si(OH)_4$ are the main aqueous species of Ge and Si under geochemical conditions relevant to ore formation. F^- and SH^- complexes may be significant when their affinities are high. Sphalerite, quartz, and topaz are proposed as final host minerals. This study explores how these ligands and crystals influence Ge-Si partitioning using thermodynamic integration based on ab initio molecular dynamics simulations at pressures and temperatures near the magma source, in supercritical hydrothermal solutions, and in environments similar to sphalerite. In sphalerite, Ge(IV) is thought to replace Zn(II), creating charge and size mismatches in the crystal structure, which has generated debate about its incorporation mechanism. To explore this issue, atomistic simulations are employed to evaluate potential pathways for germanium substituting zinc in sphalerite.

Results from the first phase of the simulation indicated that SH^- is the most important ligand for Ge/Si differentiation. In the second part, our findings suggest that replacing 2 Ge(IV) + 4 Cu(I) with 6 Zn(II) in sphalerite, with Ge-Ge, Cu-Cu, and Cu-Ge distances of 5.4 Å, 3.8 Å, and 3.8 Å, respectively, in an octahedral geometry, effectively balances mismatches and is energetically favorable.