

Interactions of Ba²⁺ and SO₄²⁻ with the Quartz (101) Surface Modeled via Density Functional Theory

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Heterogeneous precipitation of barium sulfate (barite) is an important geochemical process and a technological problem in the petroleum industry. The fundamental physical chemistry of this process must be understood at a molecular level in order to make predictions of behavior in the environment and to design strategies for pipe scale prevention.

This work uses periodic density functional theory (DFT) calculations in the Vienna Ab-initio Simulation Package (VASP) to model Ba²⁺ and SO₄²⁻ ions in various states at the quartz (101)-water interface. The purpose of this work is to connect the molecular structure with the thermodynamics of BaSO₄ in solution, in ion pairs near a surface and as a precipitate on the surface.

Models of Si₇₂O₁₄₄ + 4Ba²⁺ + 4SO₄²⁻ + 57H₂O and Si₂₁₆O₄₃₂ + 2Ba²⁺ + 2SO₄²⁻ + 203H₂O were constructed to investigate the relative energy differences among configurations with Ba²⁺ and SO₄²⁻ in solution, as adsorbed species both as individual ions and as ion pairs and as a monolayer of BaSO₄ on the quartz (101) surface.

Three of the four models with low relative energies exhibit ion pairing at the surface. The other low-energy model had a Ba²⁺ at the surface and SO₄²⁻ in solution. A model with a monolayer of 4 Ba²⁺/SO₄²⁻ pairs is stable with bonding between the Ba²⁺ and the O atoms of the SiOH surface groups.