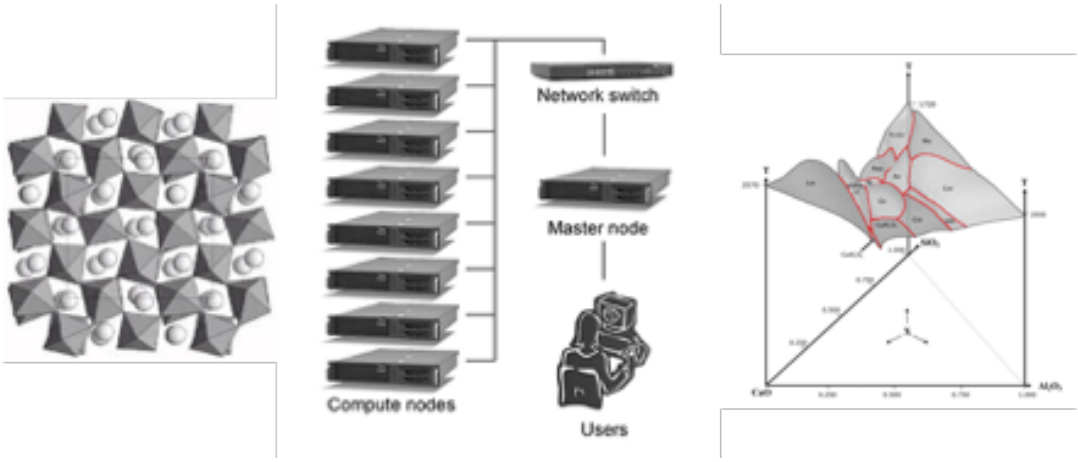
GEOCHEMISTRY

Thermodynamic and reactive properties of natural matrixes



Our research concerns mainly with minerals, liquids and glasses, aqueous solutions and gases. Through first principles (ab-initio calculations) we determine the various thermodynamic and thermophysical parameters of pure substances ($H°_f$, S°, V°, C_P, C_V, α, β, dK/dT, dK/dP) and their isotopic separative effects. Through applications of polymer chemistry we determine the mixing properties of chemically complex silicate liquids and compute the equilibrium hypersurfaces at liquidus (petrogenetic diagrams). *Ab-initio* calculations allow us to establish the properties of solutes in aqueous solutions and their behavior related to mineral phases building the porous media framework in reservoir and aquifers. Through the adoption of *real-time* mapping procedures (acquired through extensive adaptive and data-driven sampling survey) we produce elemental maps of our national territory at different scales.

Keywords: geochemistry, thermodynamics, computation

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