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From planetary surface spectroscopy to deep interiors in a numerical lab: atomistic first-principles simulations

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We highlight applications of first-principles calculations based on density-functional theory, density-functional perturbation theory and molecular dynamics. We present intuitively the background of the various calculations. We exemplify with investigations of the physical behavior of major planetary materials under extreme conditions, currently unreachable in experiments: the phase diagram of the (Fe,Mg)SiO_3 perovskite and post-perovskite system; the phase diagram of H_2O ice; the electrical conductivity of iron in planetary cores. We briefly present the WURM project on theoretical mineral spectroscopy as a model for sharing numerical data obtained by mineral physicists with planetary scientists interested in surface mineralogy.