Stability of Iron Compounds with Uranium Impurities in the Earth's Core

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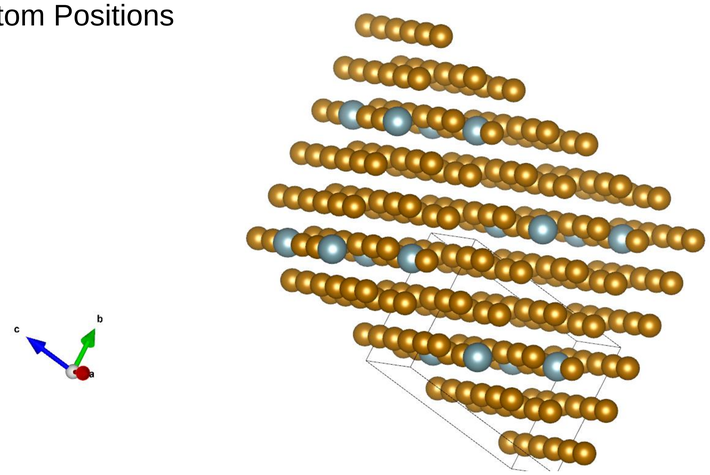
Abstract:
The composition of Earth's core is not fully understood. Specifically, it is unanswered whether or not Iron compounds are stable at various pressures. In our project, we are investigating the stability of Iron compounds of differing geometries with Uranium impurities at a range of pressures found in the Earth's core. Specifically, we are applying software, VASP, to perform relaxation calculations in which the geometries are slightly changed and the total enthalpy of the system is calculated using density functional theory. VASP wants to minimize this enthalpy, telling us what the most probable compound is. With the lowest enthalpy at hand, we can deduce the overall spontaneity of a compound forming, and we can create a convex hull that tells us the stability of such a compound. When an Iron Uranium compound forms, the convex hull tells us if it will stay a compound or dissociate into a more stable compound, such as pure Iron. With this information, we will learn more about the relative abundance of compounds in the Earth's core. Such predictions can be tested through data acquired by seismic waves. Furthermore, it can provide further insight into the formation of Earth by comparing results with what is present in meteorite samples. The project is currently still running, but is well underway.

First Step:
Atom Positions



This is a visualization of an Iron compound with Uranium impurities. The locations of the atoms are stored, and we input this file (visualization through VESTA) into VASP to do our calculations. Using the locations of the atoms and a pseudopotential, VASP calculates the entropy of this sample. Different geometries of atoms yield different enthalpies.

Second Step:
Computation

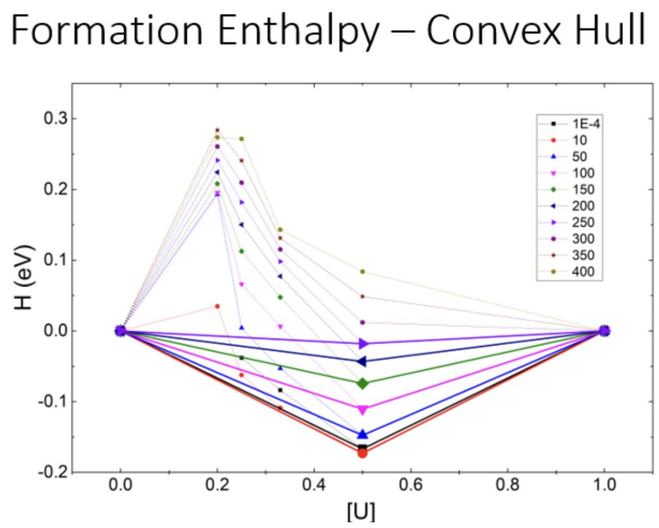
$$\hat{H}\Psi = E\Psi$$

$$\hat{H} = \sum_{i=1}^{N}\left(-\tfrac{1}{2}\nabla_i^2\right) + \sum_{i=1}^{N} v(\mathbf{r}_i) + \sum_{i<j}^{N}\frac{1}{r_{ij}}$$

$$v(\mathbf{r}_i) = -\sum_{\alpha}\frac{Z_\alpha}{r_{i\alpha}}$$

This is the Schrodinger equation, the fundamental equation of Quantum Mechanics. VASP uses this equation when it does calculations. The potential term makes solving the equation exceedingly difficult, if not impossible, to solve analytically. Thus VASP uses pseudopotentials and numerical techniques to solve the equations.
Equations from Density-Functional Theory of Atoms and Molecules, Robert G. Parr and Weitao Yang

Third Step:
Interpret Results



This is an example of a convex hull, with the enthalpy of formation on the y-axis and the Uranium content on the x-axis (Botana, McGarvey, Gilbert). The convex hull plots the enthalpy of formation of a compound as a function of Uranium concentration and pressure. Each point corresponds to a different pressure. It allows us to deduce the spontaneity of compounds, if they will form or not, and if they are stable.

Future Steps:

- Continue optimizing parameters such as KPOINTS (accuracy of calculation), to minimize enthalpy.
- Run relaxation scripts to find the total enthalpy of the system given a pressure.
- Get sufficient data to create a convex hull showing enthalpy as a function of Uranium concentration and pressure.
- From the convex hull, deduce whether compounds of Iron with Uranium impurities are stable within the Earth's inner core.

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