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HP_MAT Project: Open-Web Based Access for High-Pressure Materials

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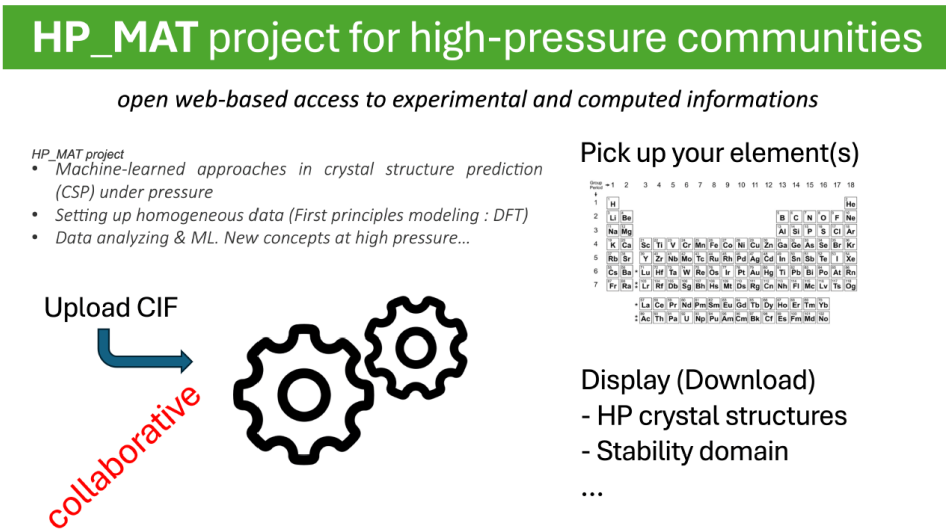
To accurately describe the behavior of planets and exoplanets, a comprehensive understanding of matter, including atomic arrangements and chemical compositions, is essential. Pressure levels vary significantly, ranging from approximately 1 atmosphere ($\sim 10^{-4}$ GPa) at Earth's surface to ~360 GPa at its core. The crystalline structure of a solid element or compound changes under pressure. This leads to the emergence of new concepts and rules in high-pressure physics and chemistry, driven by phase transitions, structural rearrangements, and novel chemical bonding. While databases for crystalline structures at standard conditions exist, there is currently no open database specifically for structures under high pressure.

Our **HP_Mat** project aims to address this gap by collecting high-pressure crystalline structures. The data will be sourced from published experimental and predicted crystals. We will also predict phases through numerical simulations using Crystal Structure Prediction (CSP) codes, an area in which our IC2MP research group possesses relevant expertise. We plan to use evolutionary algorithms coupled with machine-learned potentials to accelerate the scanning of a compound's potential energy surface at a given pressure. Our objective is to locate both global and local minima. These Density Functional Theory (DFT) and machine-learned approaches will enable us to obtain homogeneous data, including accurate energies, structural parameters, elastic and mechanical tensors, phonons, Density of States (DOS), band structures, Electron Localization Function (ELF), and other relevant physical and chemical descriptors. We intend to perform in-depth analysis of this data using machine learning techniques to develop new concepts and models suitable for high-pressure matter. Ultimately, this open science project will benefit the high-pressure and materials science academic communities by providing valuable data, including energies, structural parameters, elastic and mechanical tensors, phonons, DOS, band structures, ELF, and other relevant descriptors.



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