Legend for Supplementary Data 1

Overview

This document explains the contents of each folder and subfolder within the Supplementary Data 1 zip file. The data includes calculations and configurations related to various energy-strain calculations for materials and optimized atomic configurations.

Description: This supplementary data file, labeled "Supplementary Data 1," contains the atomic coordinates of all optimized computational models discussed in this study. Each model's atomic configuration is provided in a separate CONTCAR file within the zip archive. These CONTCAR files can be opened with any text editor (e.g., Notepad) and contain the raw data in a format that preserves the structural details of each model.

Folder Structure and Descriptions

1. Figure 5 Optimized Atomic Configuration DFT folder
    - Contains data files and subdirectories related to optimized atomic configurations using Density Functional Theory (DFT). The structure is organized by figures and specific calculations.
2. Subfolders within "Figure 5 Optimized Atomic Configuration DFT"

2.1. Figure 5b-f folder

- This folder includes subdirectories for energy-strain calculations of shear modulus values for different material configurations.
- Energy-Strain Calculation for Shear Modulus
    - Subdivided by material structure and modulus type (e.g., C11_C12_C22, C22_C25_C55, etc.).
    - Each configuration folder contains strain subfolders, labeled by strain values, each holding:
        - CONTCAR: Optimized atomic positions under a given strain.
        - STRAIN_ENERGY.dat: Tabulated energy values corresponding to each strain state.

3. Relaxed CONTCAR folder
    - Includes directories by material type and crystallographic structure (e.g., Cr2O3-167, FeNi2O4-227).
    - Each material folder contains:
        - CONTCAR: Final relaxed atomic configuration for the specific material.

File Format:

- CONTCAR: A configuration file containing atomic positions in a relaxed state.
- STRAIN_ENERGY.dat: Text file containing energy vs. strain data for a specific material and modulus type.

How to Use:

- To view the atomic coordinates, simply open any CONTCAR file with a basic text editor or import it into computational software for further analysis.
- The data format in the CONTCAR files is in plain text format. If the reader needs it in an unrestricted or simpler plain text file (such as .txt or without specific formatting constraints), one can simply rename the file from CONTCAR to CONTCAR.txt or any other desired extension:
  - **Windows**: Right-click on the file, choose "Rename," and change the extension to .txt.
  - **Linux/Mac Terminal**: Use the mv command:

    bash

    mv CONTCAR CONTCAR.txt
- The stress-strain.dat file is located in: Figure 5 Optimized Atomic Configuration DFT/Figure 5a/cr2o3-shear/stress-strain.dat can be opened using Python. Alternatively, the reader can rename the file: change *stress-strain.dat* to *stress-strain.txt* and then open the file with any text editor, such as Notepad and TextEdit.