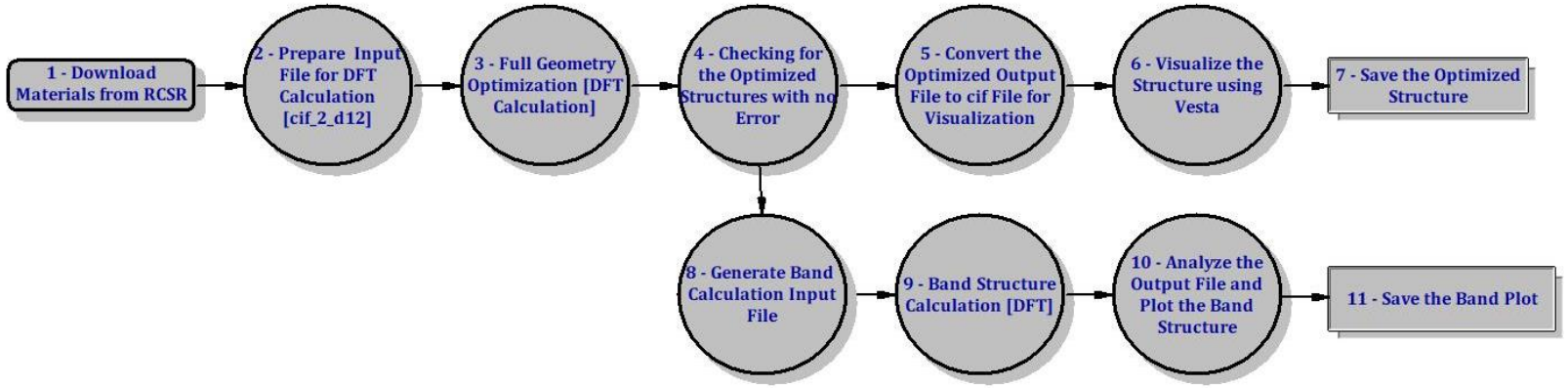
Computational workflow for Emerging 2D carbon Allotropes: A Focus on Electronic Properties

The proposed workflow will incorporate several building blocks and crystal symmetries from a known database. The workflow will span through retrieving crystal prototypes from the database, standardizing the file formats, conducting global optimization using the first-principle calculation, and investigating electronic properties. Utilizing the generated plots, a systematic classification of the novel 2D carbon materials will be performed, categorizing them as topological insulators, Weyl semimetals, or Dirac semimetals, depending on factors such as the building blocks, symmetry breakings, and space groups.



1. We have more than 100 materials extracted from the RCSR database in cif format.
2. A code is needed to convert the cif file to the input file in d12 format as needed by the DFT software.
3. DFT calculations to optimize the structure parameters (on HPCC).
4. A code is needed to separate the
5. A code is needed to convert the output file to a cif file for visualization.
6. Visualization can be achieved by relevant software such as Vesta.
7. Save the optimized structures.
8. For the property calculations (such as band gap), code is also needed to convert the optimized output file to a band input file.
9. DFT calculation to obtain the band properties (on HPCC).
10. A code is needed to analyze and plot the band structure.
11. Save the band plot.

Summary