THE BAND STRUCTURE OF 4-D TRANSITION MAX PHASES

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OBJECTIVES

- Determine the Band structure of Max-phases using AiiDA

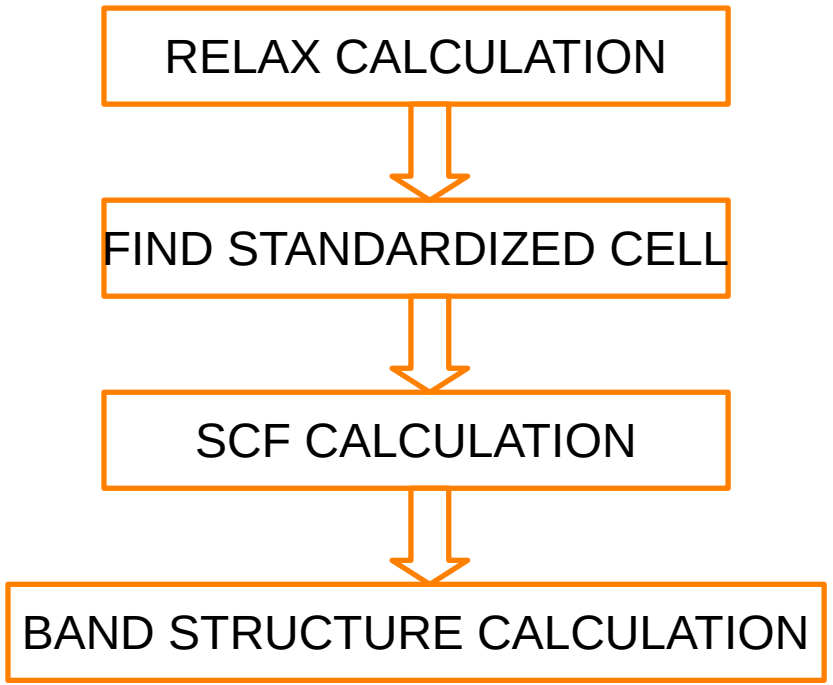
AiiDA WORKFLOW

- We utilized Quantum Espresso code and AiiDA as a Tool.
- Workfllow is a series of activities that are necessary to complete a task.

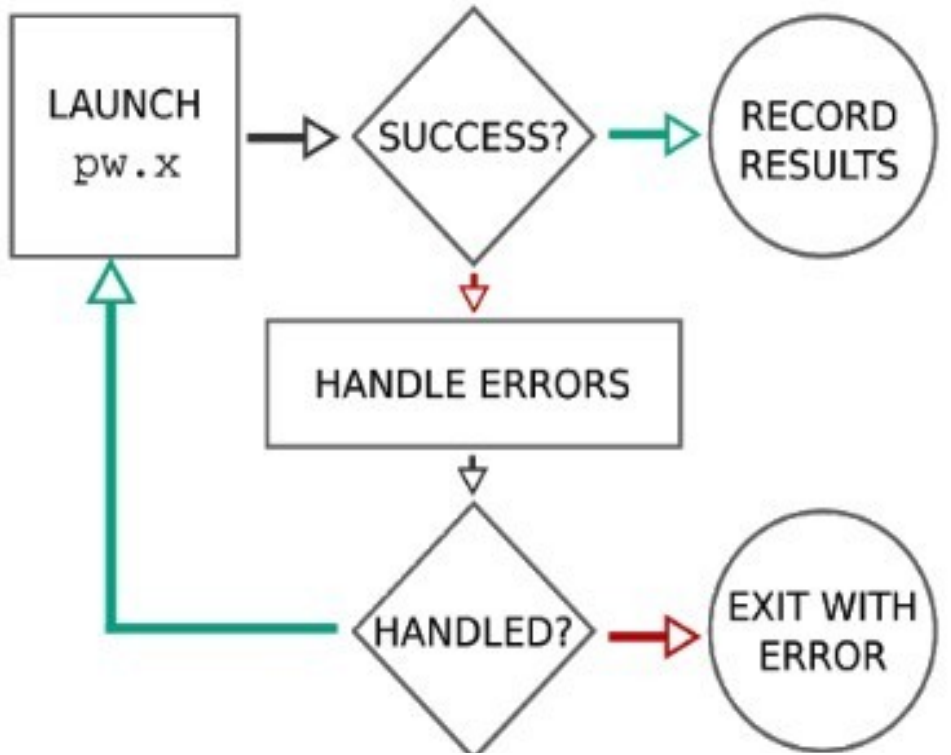
BAND STRUCTURE WORKFLOW

- Run a calculation on the cell to relax both the cell and the atomic positions (vc-relax)
- Refine the symmetry of relaxed structure, and find a standardized cell using SeeK-Path
- Run a SCF calculation on the refined structure
- Run a Band Structure calculation at a fixed kohn-Sham potential along a standard path between high-symmetric k-point determined by Seek-Path

BAND STRUCTURE WORKFLOW

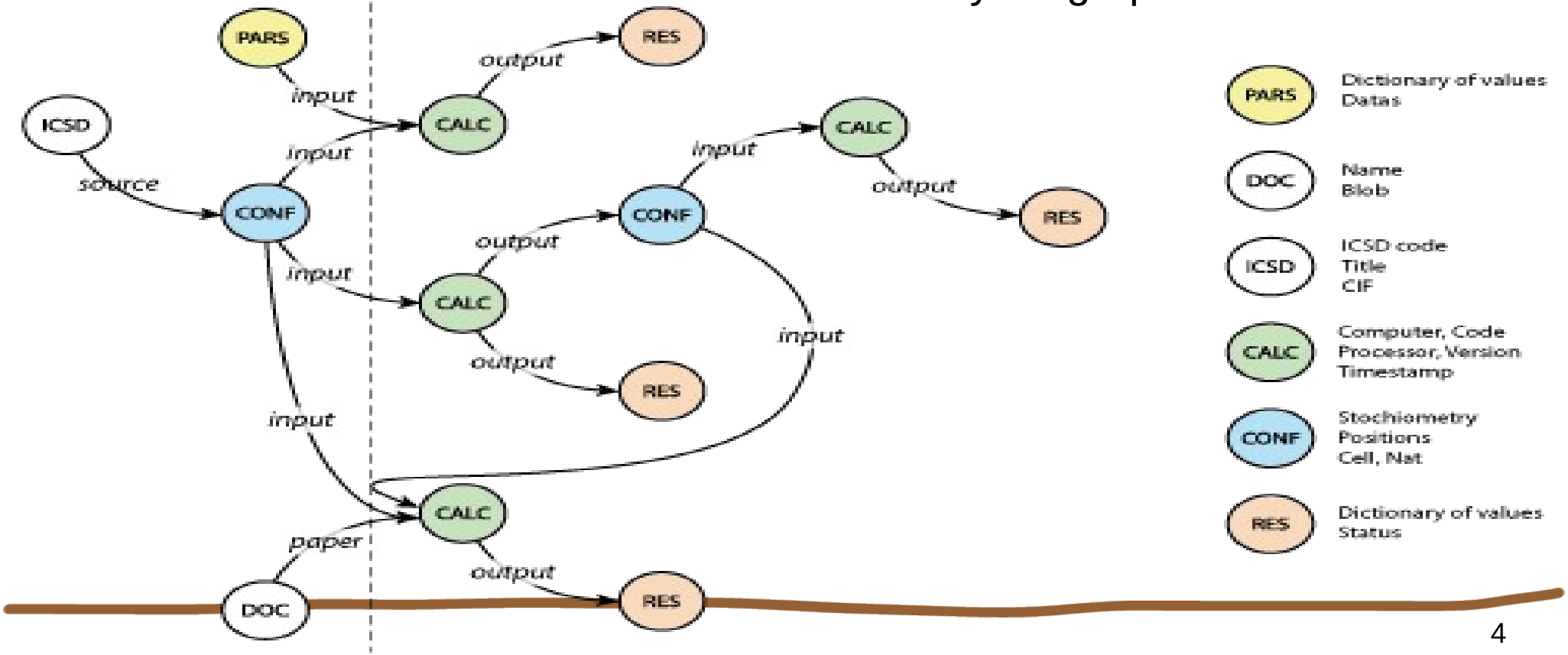


WORKFLOW ERROR HANDLING



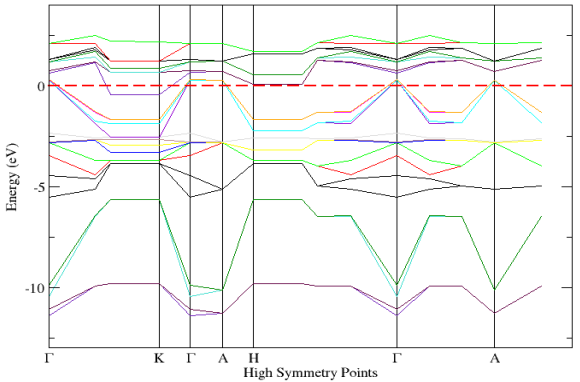
PROVENANCE GRAPH

- Data provenance in AiiDA is tracked using nodes, that is, each calculation has a node that connects its input and output data nodes, therefore data is saved in form of a direct acyclic graph.

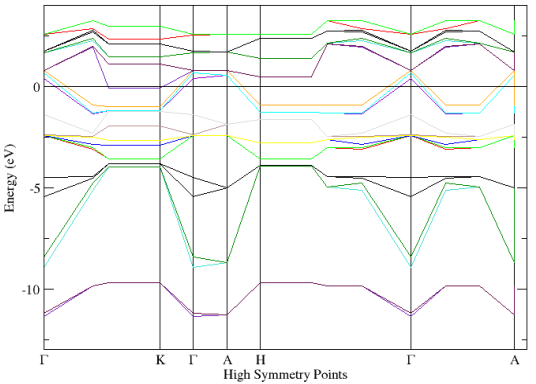


RESULTS

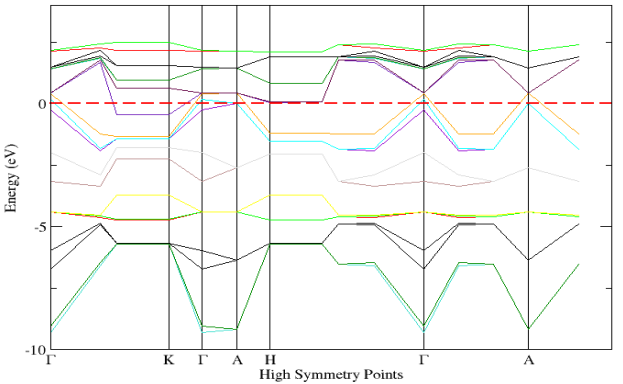
Ti2SnC BANDSTRUTURE



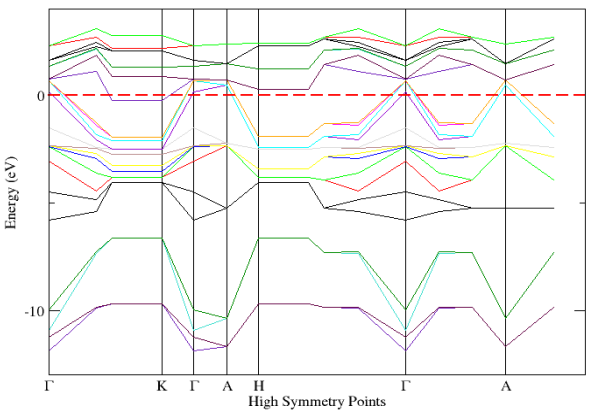
Ti2GaC BANDSTRUCTURE



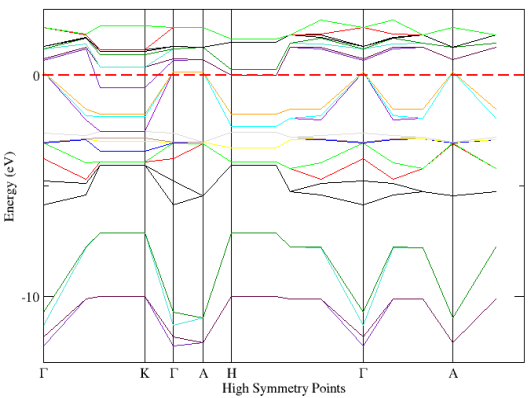
Ti2GaN BANDSTRUTURE



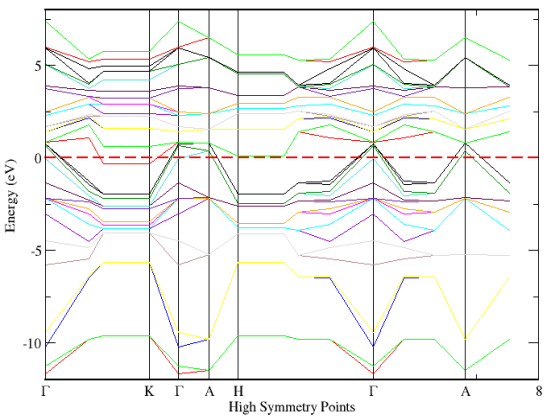
Ti2GeC BANDSTRUCTURE



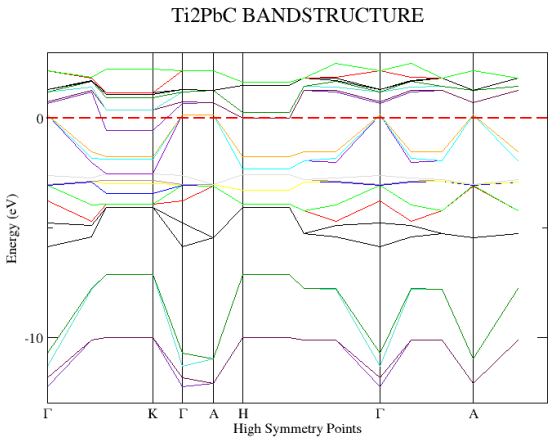
Ti2PbC BANDSTRUCTURE

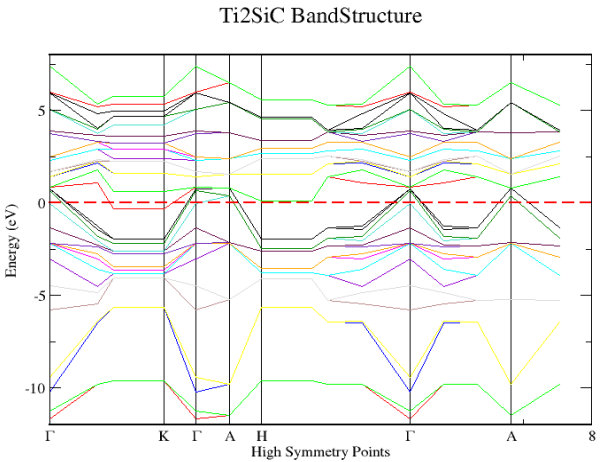


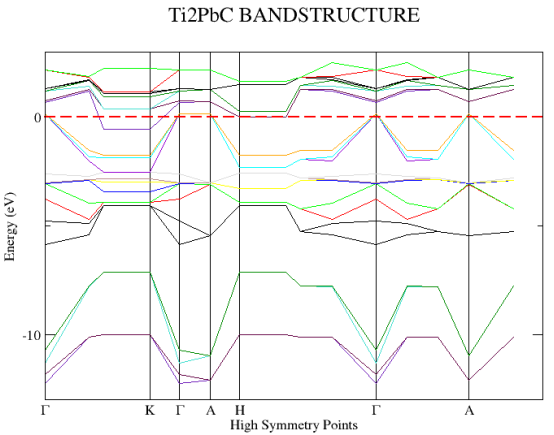
Ti2SiC BandStructure



RESULTS







CONCLUSION

- The graphs of the Max Phase band structure from the results shows that it has no direct gaps, and the band gaps is 0.00 eV, suggesting that it is all mettalic.