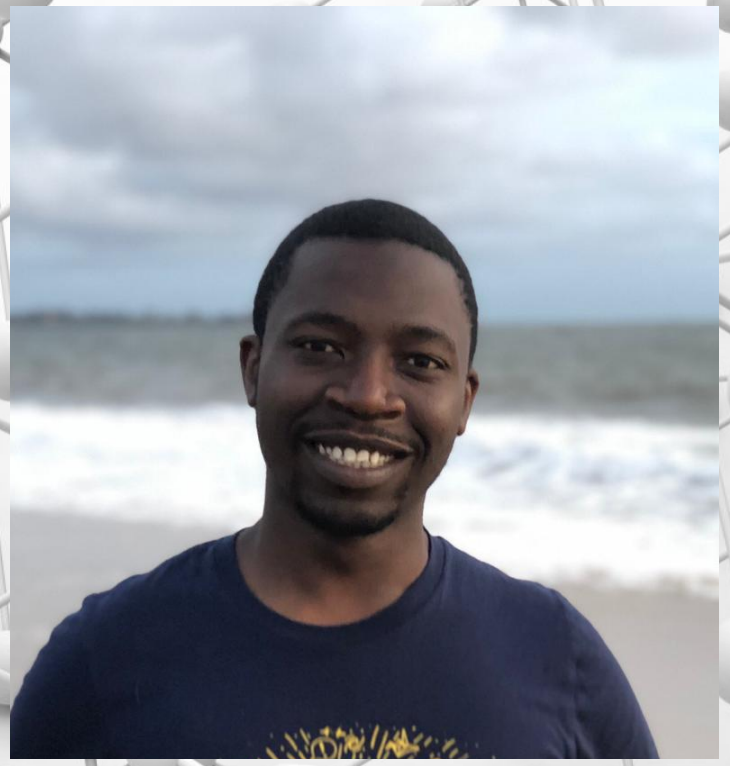
Keith Phuthi

-Did undergrad in Physics
-Currently second year PhD in Mechanical Engineering at Carnegie Mellon University

Focus is on computational material discovery i.e. using Density Functional Theory, Molecular Dynamics and applying Machine Learning to accelerate Quantum Mechanics calculations.

The materials I consider are mostly related to energy storage such as Solid Electrolyte Interfaces and Metal Hydrides



Machine Learning Potentials in place of DFT

- Relatively new field so there are not many mature and trusted blackbox codes out there, poor documentation and often suboptimal performance.
- I train various custom models across platforms like tensorflow, pyTorch etc. on HPCs and would like to optimize my training procedures as much as possible
- I write/prototype a lot of my own code for data curation/analysis and pipelines usually involving very data intensive calculations. Fast turnaround in results is important for prototyping.
- I want to be able to contribute to existing codes so I need to know that my code is decent
- I do not know if I am using my computing resources efficiently