

HBKU Thematic Research Grant 1st Cycle– Project Highlight

Project Title: An Artificial Intelligence Platform for Accelerating Materials Discovery (AIPAM)



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Executive Summary

The project aims to develop software services to create and execute computational materials science workflows, with a primary focus on the integration of data structures that follow the FAIR data principle. The team will mature tools and services required to support materials science research and develop a webservice of artificial intelligence for materials scientists. This includes the development and integration of machine-learning-driven decision-making on models as well as automated and robotics assisted materials synthesis. We aim to accelerate de-risking and maturing the AiMater© pilot platform currently under development by the LPI team. The pilot platform and its components have been disclosed and protected via copyright by the IDTK. The project will enable to make full advantage of the Accelerated Materials Discovery capabilities and assets of HBKU-QEERI and Artificial Intelligence at HBKU-CSE to translate them into licensed and marketable products and solutions. It is strongly supported by existing facilities such as but not limited to QF and HBKU IT infrastructures and laboratories. It will also benefit from the collaboration with HBKU IT for the deployment of the platform to end users using state-of-the-art cloud hosting.

Expected Outcome

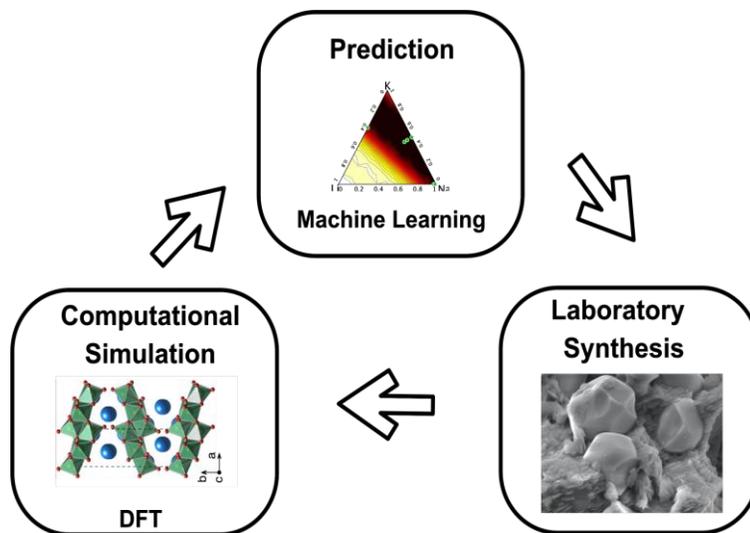
- Materials databases integrated into *Qatar Materials Database*© with a potential for licensing
- Computationally designed novel materials and processes supported by lab-scale proof of concept adaptable to the evolving economy of the State of Qatar with potential for licensing
- Innovative Machine learning predictors: Building adaptable and optimized predictive AI models for niche materials application that would enable exploring the chemical space and looking at highly performing materials and processes.
- Explore the possibility of incubation at QSTP of a software company

Collaborating HBKU entities: College of Science and Engineering-ICT

Photos:

Mixed Cation Solar cell devices optimized by the help of machine learning method

(c) Data-driven acceleration in materials discovery



ML predicted Energy landscape of a lead based and lead free perovskite

