AQTIVATE: Advanced computing, Quantum algorithms and data-driven Approaches for science, Technology and Engineering

AQTIVATE KICK-OFF EVENT

Summary of my Master's Project and previous Research work

Sachin Shivakumar

Project 14: Accelerating QM/MM simulations via machine learning
FZ Juelich, RWTH, and KTH

Funded by the European Union

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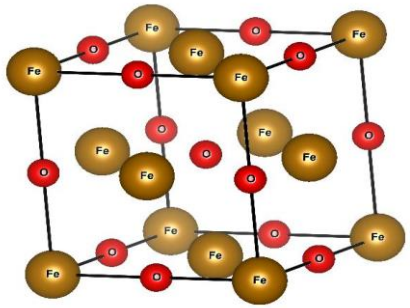
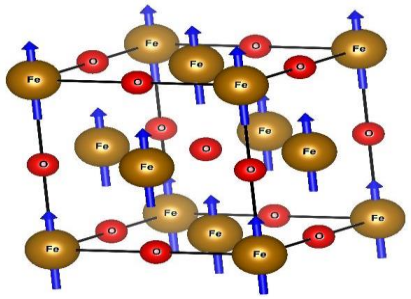
An Ab Initio Study of Structural and Electronic Properties of Si (Fd-3m) and FeO (Fm-3m) using Density Functional Theory

Goals

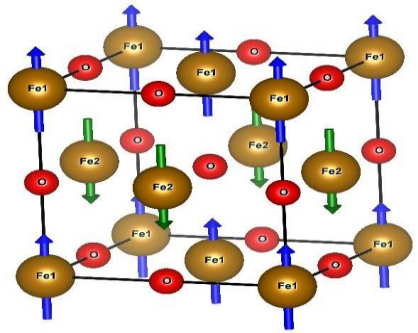
- Study mathematical formalism of DFT
- Gain experience in practical application of DFT by studying Si and FeO crystals



Non-Magnetic



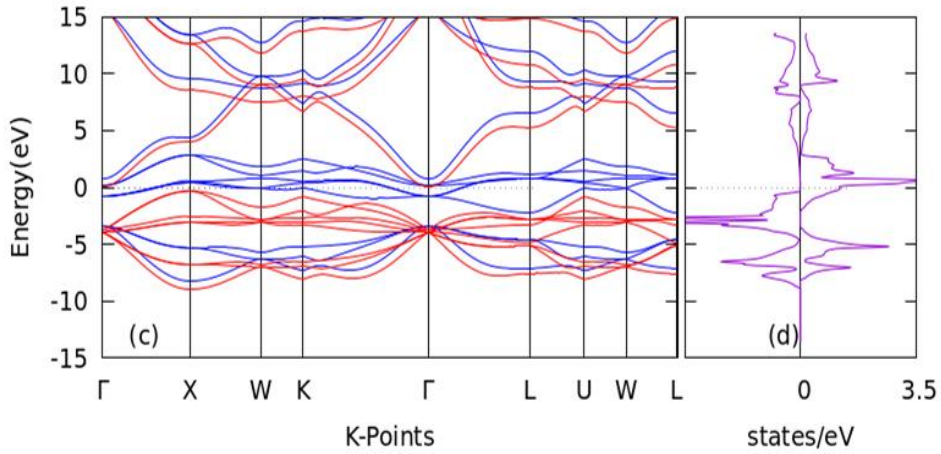
Ferromagnetic



Antiferromagnetic

- DFT code used: ELK
- Computed ground state energy, lattice parameters, band structure, PDOS and TDOS.

- Results compared between different DFT functionals (LDA vs GGA)
- Results were validated with reported experimental and simulations results



Supervisor: DR. Rajesh kumar, NIT Hamirpur, India

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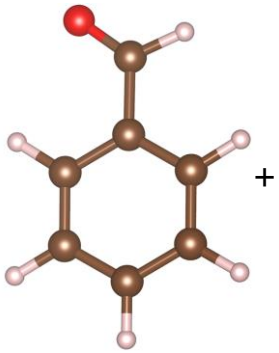
LITESOPH : Layer Integrated Toolkit and Engine for Simulations of Photo-induced phenomena

Application in Photovoltaics, Water-splitting catalysts, opto-electronics.



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- TDDFT codes
- parameters
- programming
- experience in linux
- submit job
- monitor job
- extract data
- post processing
- visualizations

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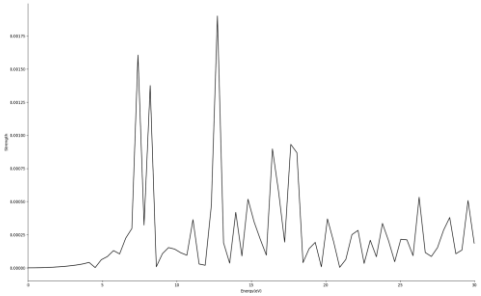
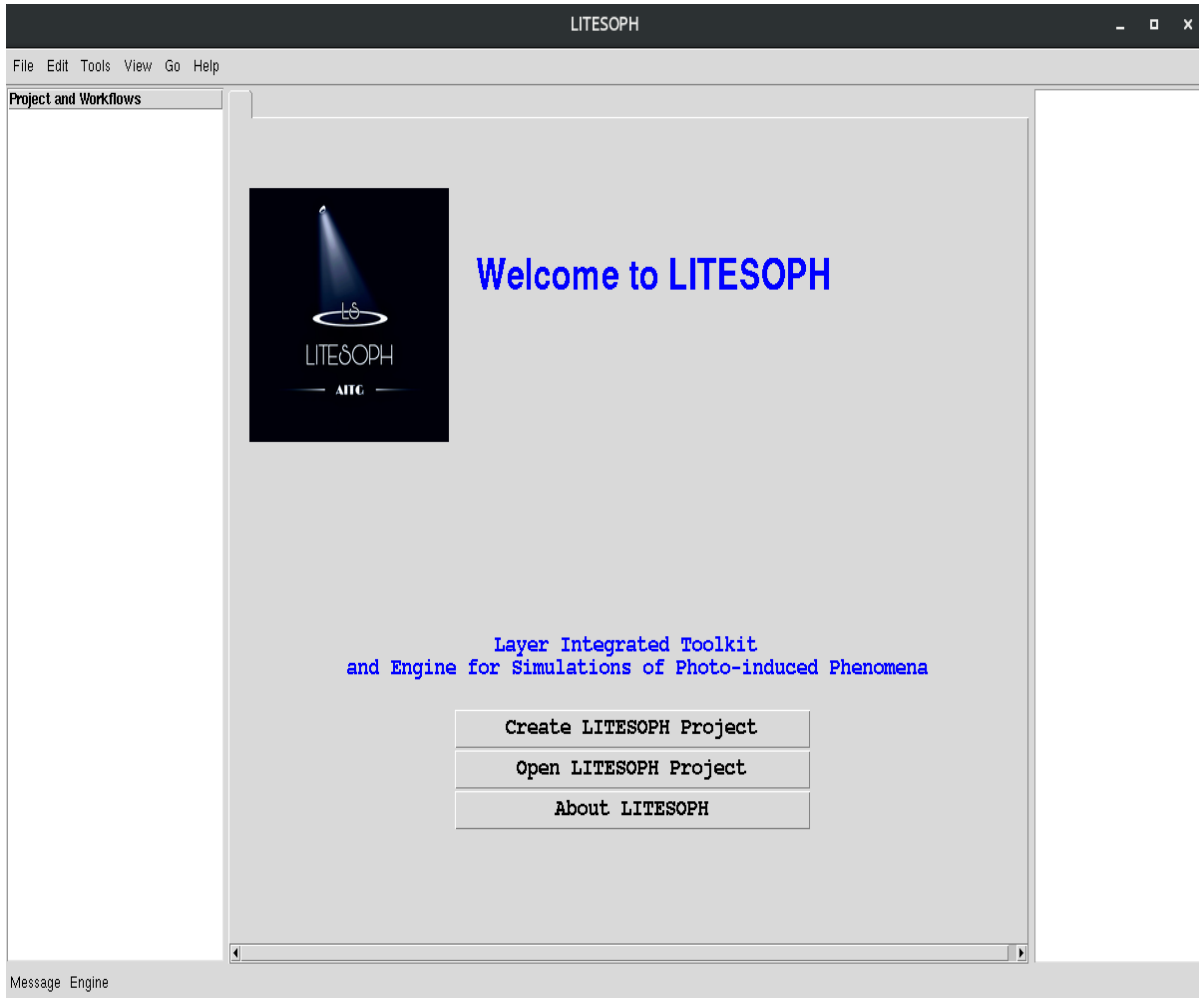


spectrum



PI: Dr Varadharajan Srinivasan
IISER BHOPAL,
Funding: CDAC PUNE (NSM)
https://aitgcodes.github.io/litesoph-website/index.html

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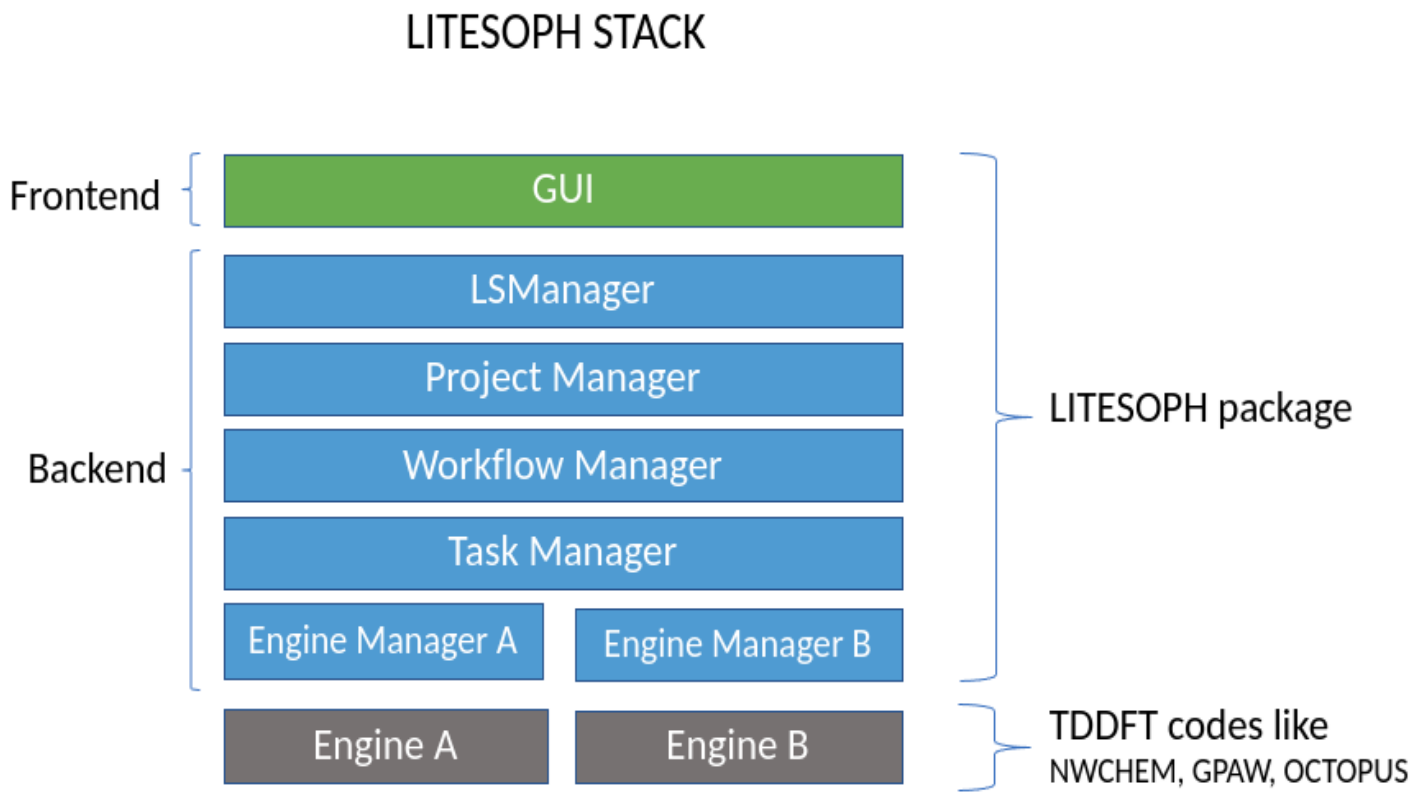
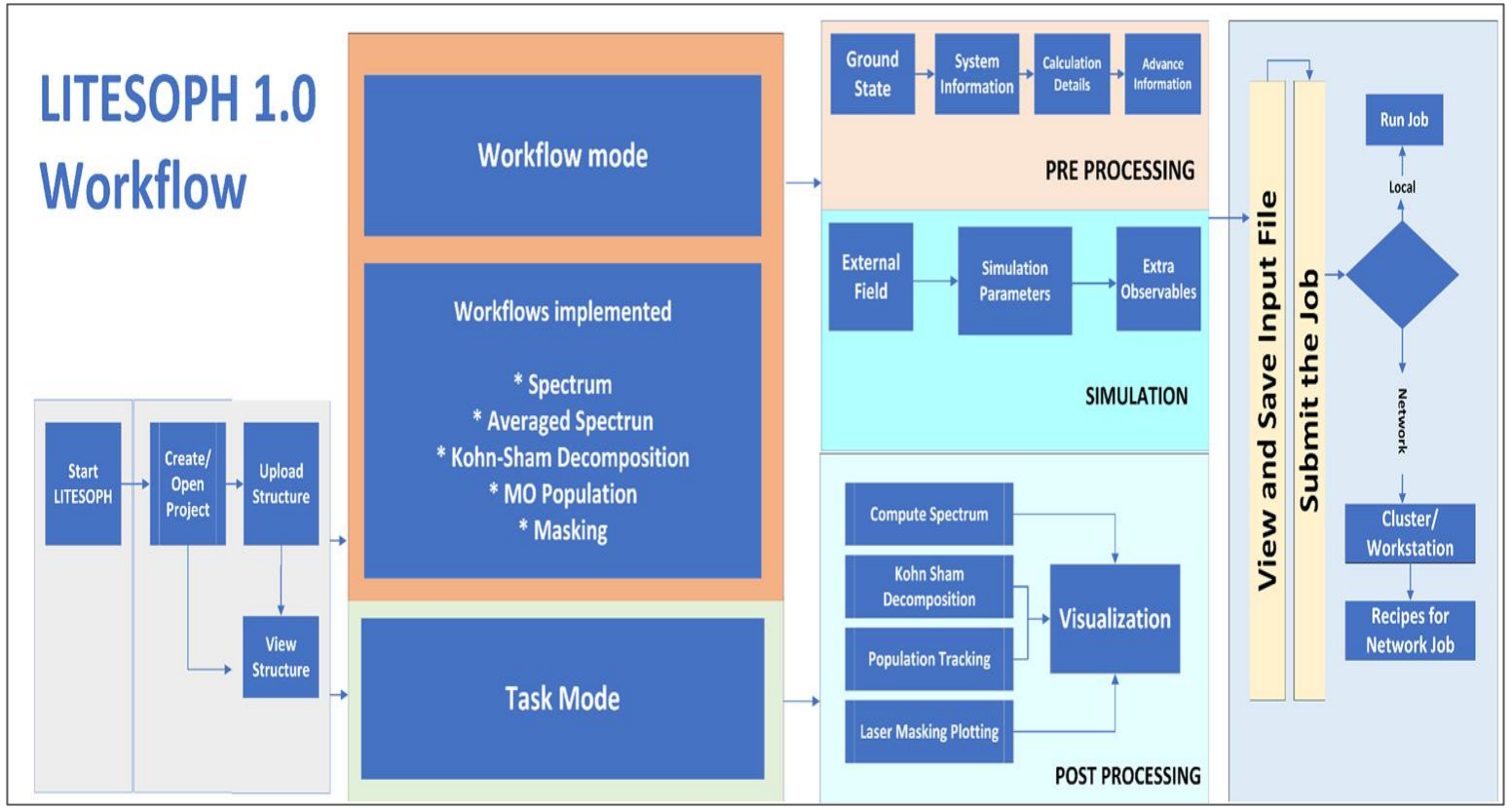
Design Principles of LITESOPH

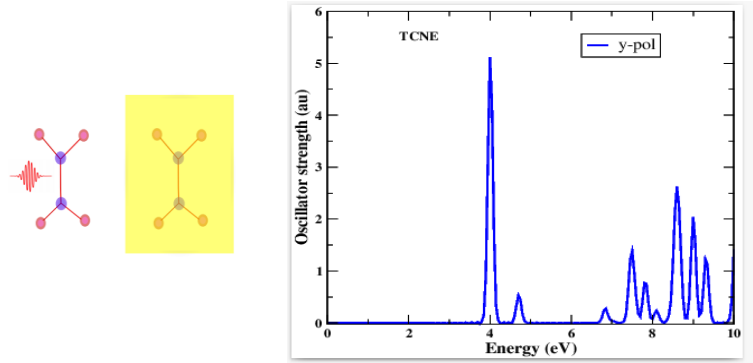
- Maintainability (faster debugging)
- Extensibility (easy to add new features)
- Understandability (easy to collaborate and faster development)

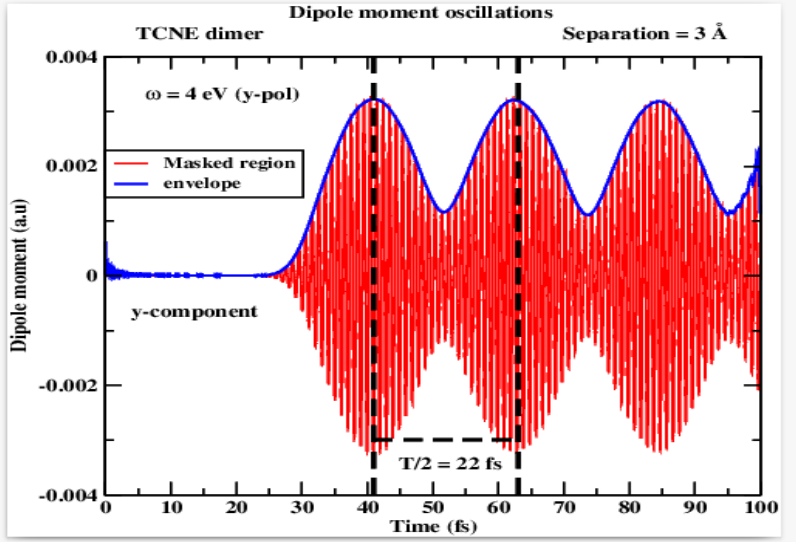


LITESOPH: Features and Functionalities



Energy Transfer TCNE*





*Dr. Pramod Verma, R.A
Ilser Bhopal

Accelerating QM/MM simulations via machine learning

- Enzymatic reactions,
- Transition metal binding to proteins,
- Proton Transfer, and
- Photophysical Processes

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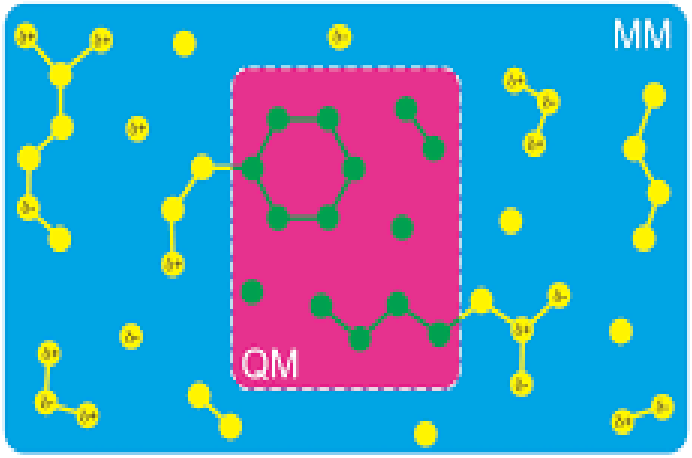
- Energy-efficient manufacturing,
- Drug design,
- High-density and Long-lasting batteries, and
- efficient solar cells.

Track electronic and atomic motions , system size > 10000

MM methods can't dynamically describe electrons.
QM methods not feasible or not possible for systems size > 10000

Currently state of art method for studying these systems is a
multiscale approach (QM/MM).



The QM/MM approach treats the active site of the system, where electron dynamics are crucial, at the QM level while using classical force fields (MM) to describe the rest.

- Commonly DFT is used at the QM level

http://cmb.bio.uni-goettingen.de/pract/p7/

Accelerating QM/MM simulations via machine learning

DFT QM/MM can access few hundred ps with ~ 100 QM atoms [1]

Limited sampling for free energy estimation.

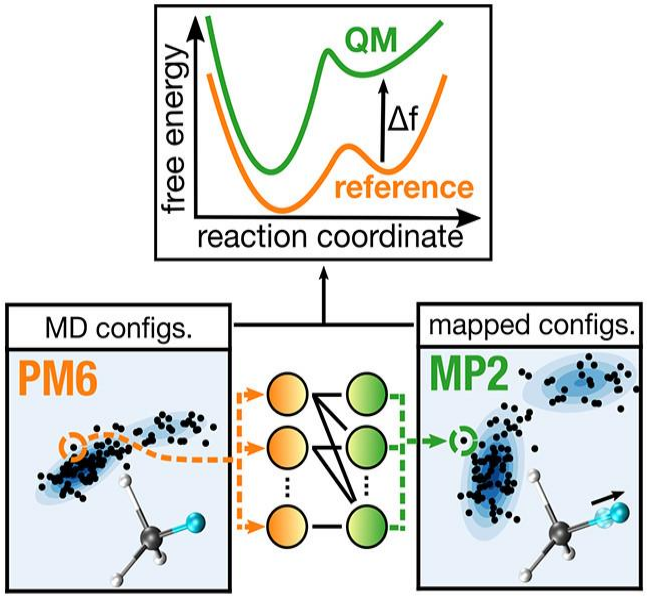
This high computational cost of DFT QM is reduced using machine learning [2]

DFT QM/MM ⟶ ML/MM

By using targeted free energy perturbation (TFEP)

Reference potential + small number of single point calculations + ML = QM potential [3]

The focus of the PhD will be to build better ML models and come up with data-efficient strategies to train these models.



[1]https://pubs.acs.org/doi/10.1021/acs.jcim.3c00557
[2]https://pubs.rsc.org/en/content/articlelanding/2021/sc/d1sc02742e
[3]https://pubs.acs.org/doi/10.1021/acs.jpclett.1c02135

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LITESOPH: PI: DR. Varadharajan Srinivasan, IISER Bhopal, India
https://aitgcodes.github.io/litesoph-website/index.html
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Dr Davida Mandelli (Researcher), Dr. Andrea Rizzi (Postdoc)
Institutions: FZ Julich, RWTH Aachen, KTH sweden.
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Thank you