



Libra: The Modular Software for Nonadiabatic and Quantum Dynamics

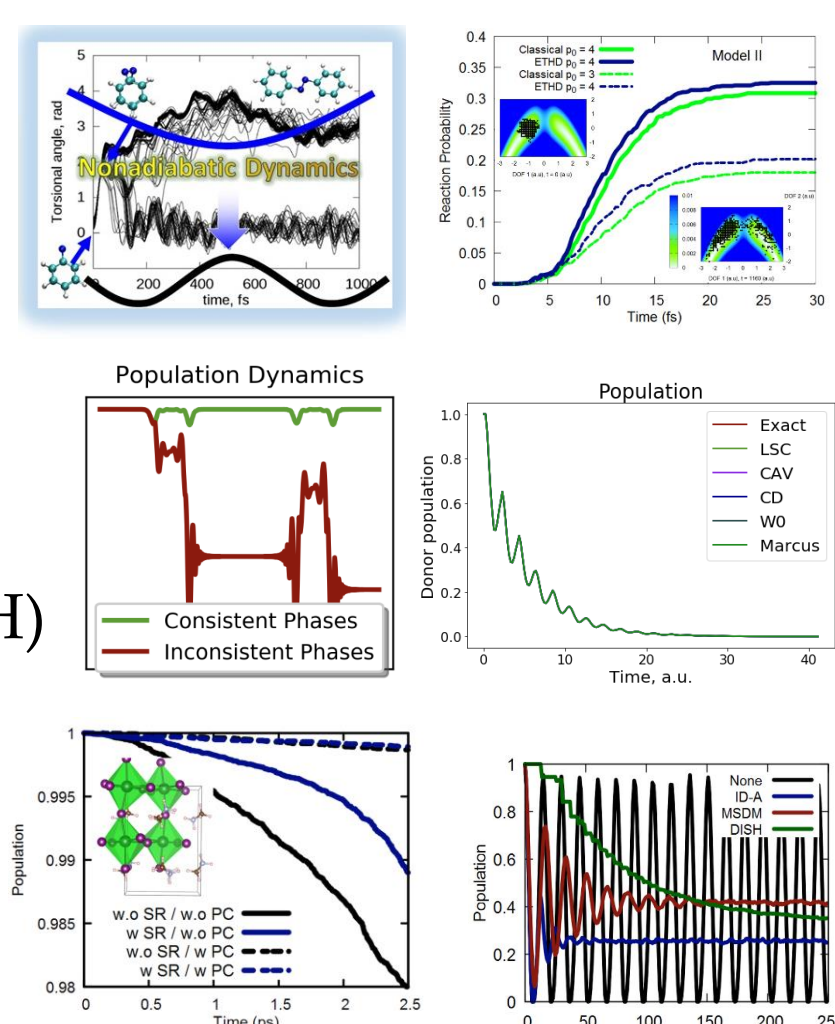
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Award #: NSF-OAC-1931366

Motivation

- Modeling of nonadiabatic (NA) and quantum dynamics (QD) in complex systems relies on approximations.
“*which method to choose?*”
- Various codes exist:
“black-box” style, not suitable for methodology development, difficult to use, redundant, inconsistent
“*library of methodology prototyping building blocks*”

To date

<https://github.com/Quantum-Dynamics-Hub/libra-code>

Nonadiabatic dynamics:

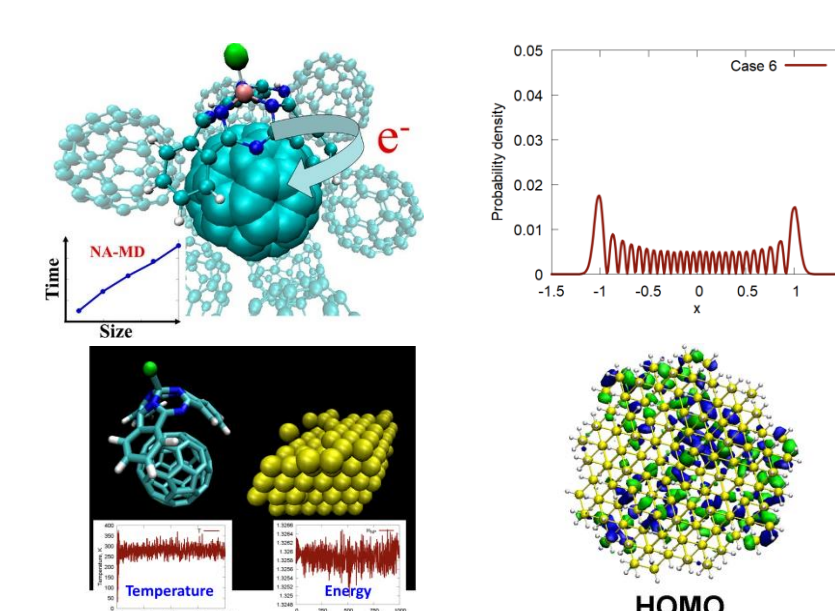
- Exact, DVR (Colbert-Miller), SOFT
- Ehrenfest
- FGR, HEOM
- TSH (FSSH, GFSH, MSSH, BCE)
- Decoherence (mSDM, EDC, ID-A, DISH)
- State tracking, phase corrections, etc.

Models Database: Tully, Holstein, Eckart barriers, SSY, Henon-Heiles, etc.

Interfaces: ErgoSCF, Quantum Espresso, DFTB+, GAMESS, Psi4

Auxiliary simulation tools:

- Semiempirical MO calculations
- Arbitrary sitribution sampling
- Classical MD (force fields)
- Analysis and data management tools



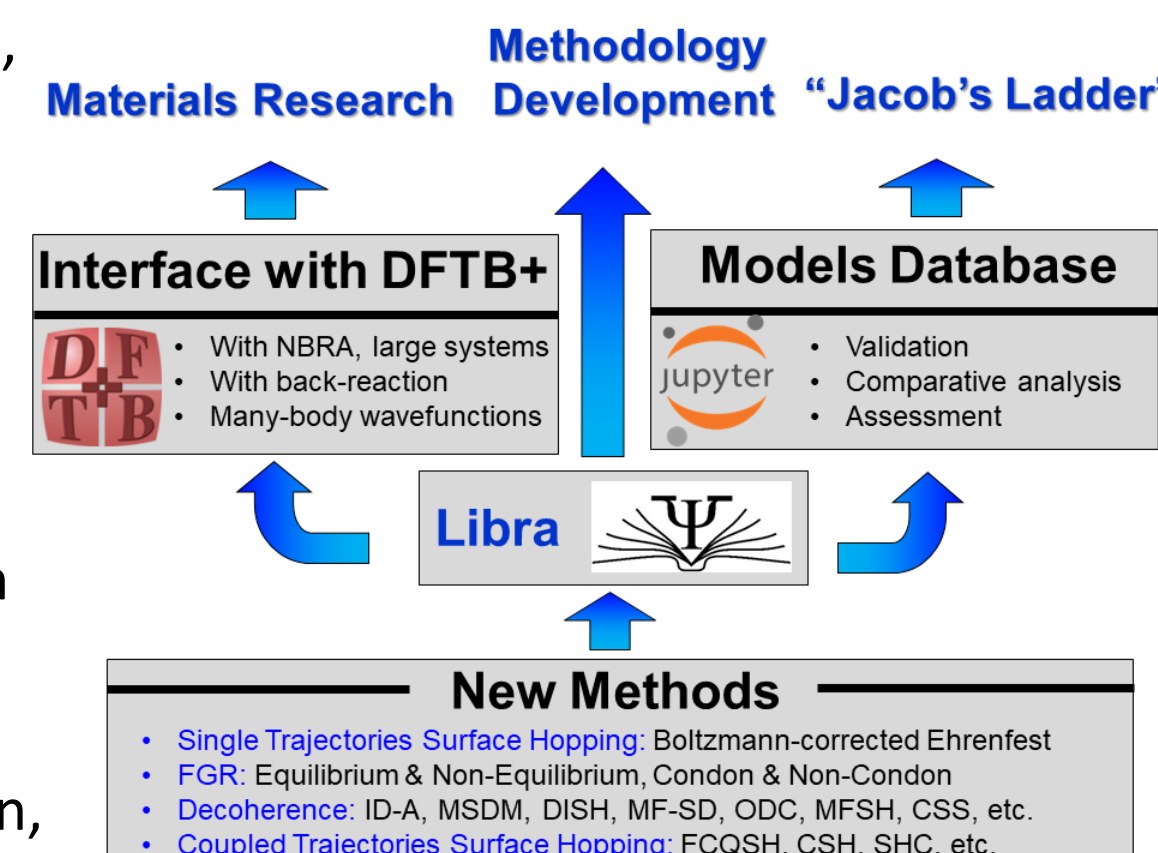
Objectives

- To develop Libra library: TSH, FGR, decoherence, coupled trajectories
 - To develop new tools: Libra/DFTB+ codes to enable modeling of nonadiabatic dynamics in nanoscale systems.
 - To systematically benchmark NA/QD schemes: build the “Jacob’s ladder” of nonadiabatic dynamics methods
- Systematic packaging/validation (HEOM, FGR, DVR)
 - Unified data handling and processing (HDF5)
 - Validating the models database
 - New decoherence schemes
 - Stochastic Schrödinger equation solvers
 - Coupled trajectories methods
 - Testing and validation of new interfaces (with ErgoSCF, DFTB+, Psi4, eQE)
 - Comprehensive comparative analysis of the methods (TSH with and without back-reaction, bath models, performance in systems with multiple DOFs)



Story Temen

In Progress



Intellectual Merit

- “Which method to choose?” Systematic assessment of approximations
- Modular software to study and develop new methods
- Enable modeling of nonadiabatic processes in nanosystems

Broader Impact

- Stimulate the adoption and re-use of advanced methods and codes
- New tools for excited states dynamics
- Provide advanced training via workshops and online open-source educational materials



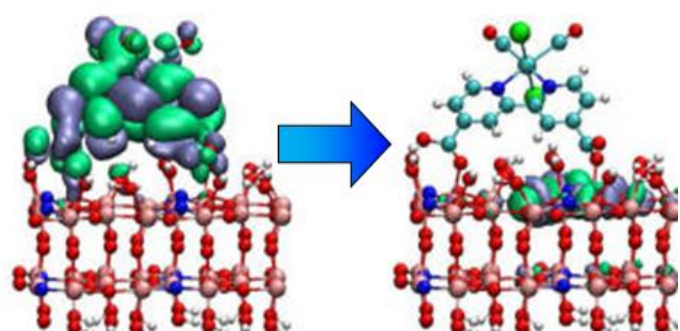
CyberTraining: Pilot: Modeling Excited State Dynamics in Solar Energy Materials

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Award #: NSF-OAC-1924256

Motivation

- Solar energy materials research
- Charge & energy transfer



- Advanced theories and methods of nonadiabatic (NA) and quantum dynamics (QD) are required.
- A plethora of tools exists
- Mastery in this cyberinfrastructure (CI) is needed

Objectives

- To develop VIDIA science gateway with tools for NA/QD.
- To provide training for graduate students on modeling excited states in materials via advanced CI NA/QD calculations



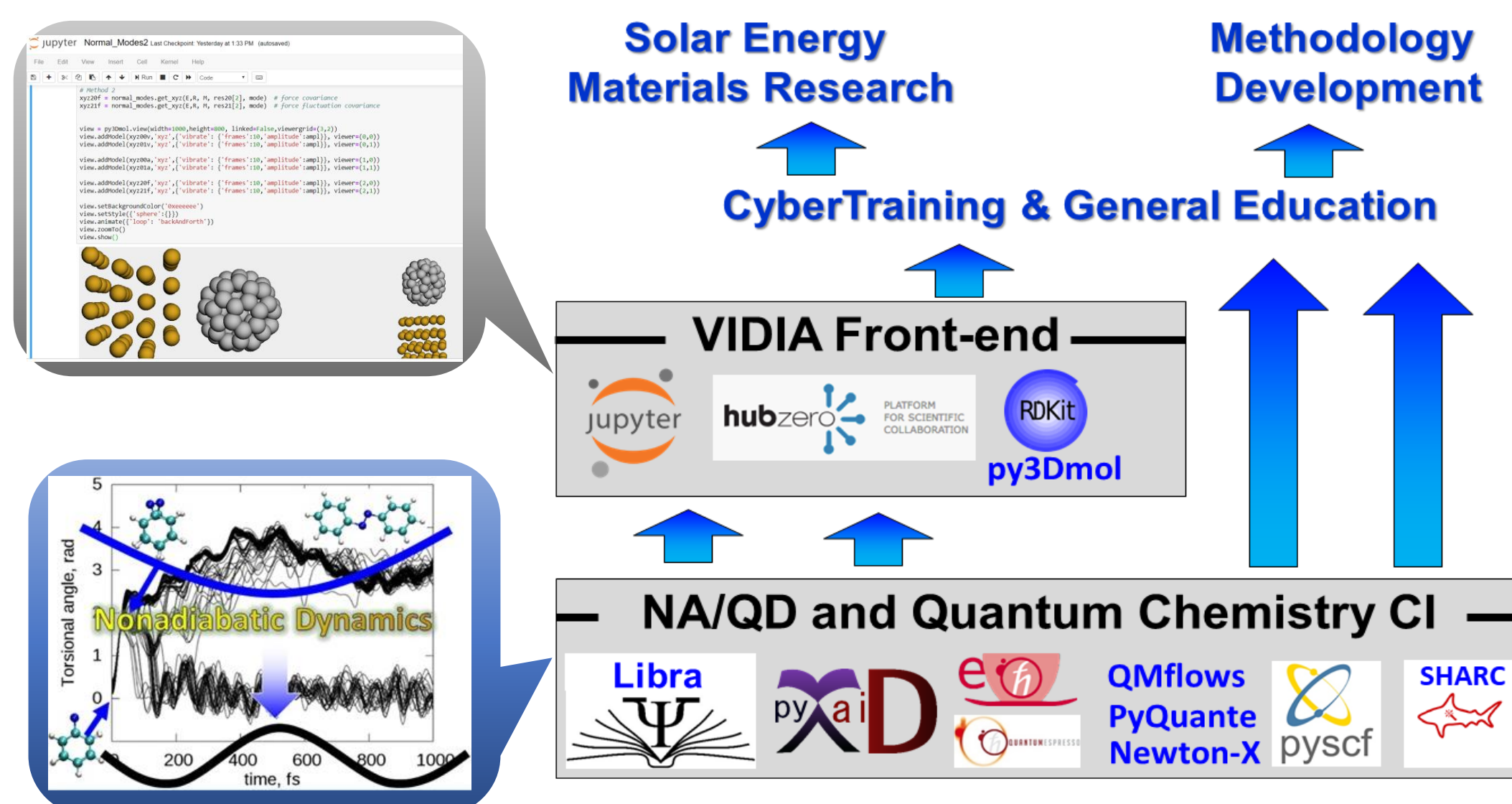
Brendan Smith

Intellectual Merit

- Promote open-source CI for modeling excited states dynamics
- Enable new science via adoption of new/advanced methods and tools

Broader Impacts

- Directly train 50 students from US institutions
- Provide a broader training via open-source educational materials
- Enable broader access to advanced NA/QM tools via VIDIA gateway
- Enable new classroom teaching approaches



Tools to Cover

Dynamics Packages:

- Libra, Pyxaid (Akimov)
- SHARC (Gonzalez)
- Newton-X (Barbatti)
- QMflows-NAMD (Infante)
- NEXMD (Tretiak)
- more to come ...

Related Electronic Structure Packages:

- Quantum Espresso, eQE
- CP2K, GAMESS
- Psi4, PySCF, ErgoSCF
- COLUMBUS
- DFTB+

- Python, terminal, Jupyter, Git/GitHub, best practices, visualization & auxiliary
- General algorithms and methods:
 - MD, integrators, TD-SE
 - Exact dynamics on the grid, DVR, HEOM, FGR
- Surface hopping
 - Models Hamiltonians
 - Interfaces with electronic structure packages
- Niche-specific materials modeling tools
 - Large systems, condensed matter, nanoscales (Libra, Pyxaid, QMflows-NAMD)
 - Large organic systems (NEXMD, Newton-X/DFTB+)
 - Clusters & Molecules (SHARC, Newton)
- Analysis & post-processing

UB Virtual Infrastructure for Data-Intensive Analysis (VIDIA)

<https://vidia.ccr.buffalo.edu/>

Software Tool	Description
RapidMiner	Workflow-based environment for data and text mining and machine learning.
RStudio	Interactive development environment (IDE) for the R language offers statistical analysis libraries.
SPSS	GNU version of IBM's SPSS software enables analysis of sampled data.
Jupyter	Notebook-based numerical computing and visualization for Python, Octave, and R.
Workspace	Linux desktop with compilers, scripting languages, and access to the user's home directory on VIDIA.

Workshops