



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

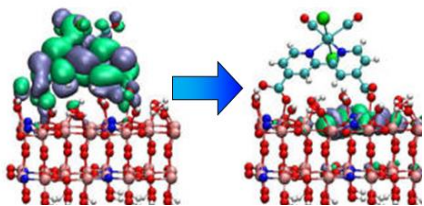
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Award #: NSF-OAC-1924256

NSF programs: CyberTraining - Training-based, OFFICE OF MULTIDISCIPLINARY AC, DMR SHORT TERM SUPPORT, Chem Thry, Mdls & Cmptnl Mthds

Motivation:

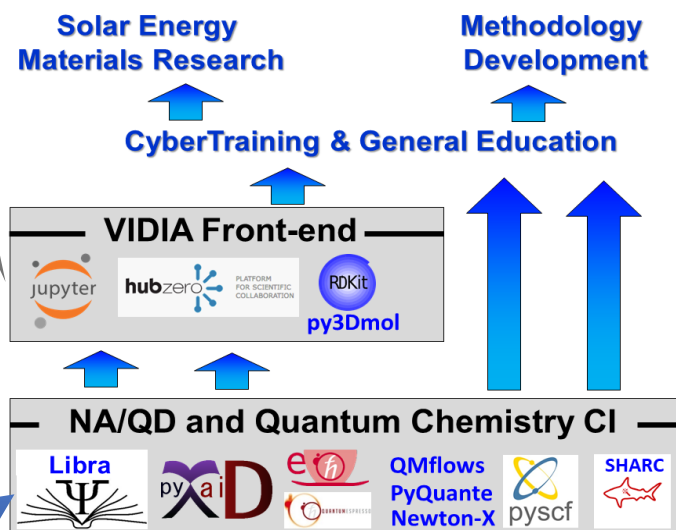
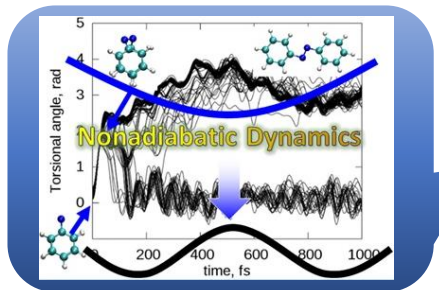
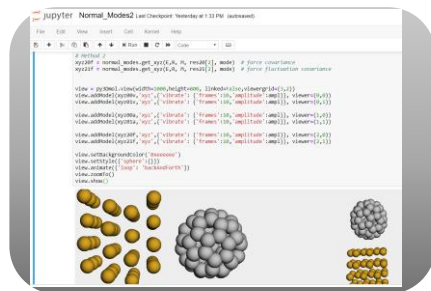
- Solar energy materials research
- Charge & energy transfer



- Advanced theories and methods of nonadiabatic (NA) and quantum dynamics (QD) are required.
- A plethora of tools exists
 - Libra, Pyxaid, Newton-X,
 - SHARC, QMflows-NAMD,
 - NEXMD,...
 - Horton, Psi4, PySCF,
 - COLUMBUS, DFTB+, CP2K, ...
- 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



Intellectual Merit:

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

Broader Impact:

- 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