CSSI Element: Libra: The Modular Software for Nonadiabatic and Quantum Dynamics

PI: <u>Alexey Akimov</u>

Institutions: University at Buffalo, SUNY

Motivation:

- Modeling of nonadiabatic (NA) and quantum dynamics (QD) in complex systems relies on approximations.

  - Surface hopping, Ehrenfest, independent trajectories, neglect of back-reaction, classical nuclei, bath models, thermal effects, decoherence, technical: state tracking, phase corrections, etc.

  "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"

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

Intellectual Merit:

- Answer the "Which method to choose?" Systematic assessment of approximations

- Modular software to study and develop new methods

- Enable efficient modeling of nonadiabatic processes in nanosystems

Broader Impact:

- <u>Nonadiabatic dynamics</u>: stimulate the adoption and re-use of advanced methods and codes

- <u>Materials research</u>: new practical tools for excited states dynamics

- <u>Education</u>: Provide advanced training via workshops and online open-source educational materials