Building a nanoHUB Graphical Interface for Exploring Protein Dynamics and Spectroscopy: the PigmentHunter App.

S. Ahad, C. Lin, and M. Reppert

Reppert Group, Purdue University

April 4th 2024

Acknowledgements

Dr. Mike Reppert
Assistant Professor

Chientzu Lin
Undergraduate Researcher

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- ITaP
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- Dr. Thomas Renger (transition partial charges)
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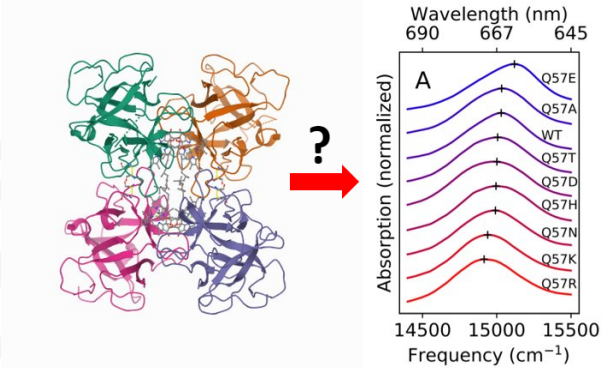
1. Background and Significance

2. PigmentHunter Interface and Workflow
   - Characterizing Pigments
   - Repairs and Mutations
   - Molecular Dynamics and Trajectories
   - Optical Spectrum from Exciton Modelling

3. Applications and Examples

Motivation

Understanding the connection between protein-pigment complex structure and optical function is complicated, making it difficult to design PPCs.



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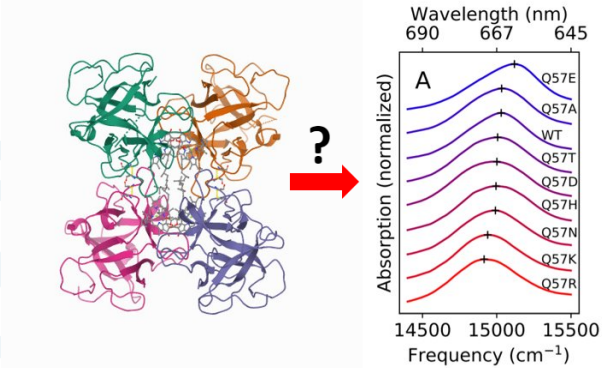

Calculating optical spectra and running molecular dynamics for proteins by hand can be tedious and time consuming.

Checklist:

- User Friendly Graphical Interface
- Doesn't require software installation
- Molecular Dynamics
- Optical Spectrum Predictions
- Computationally Inexpensive

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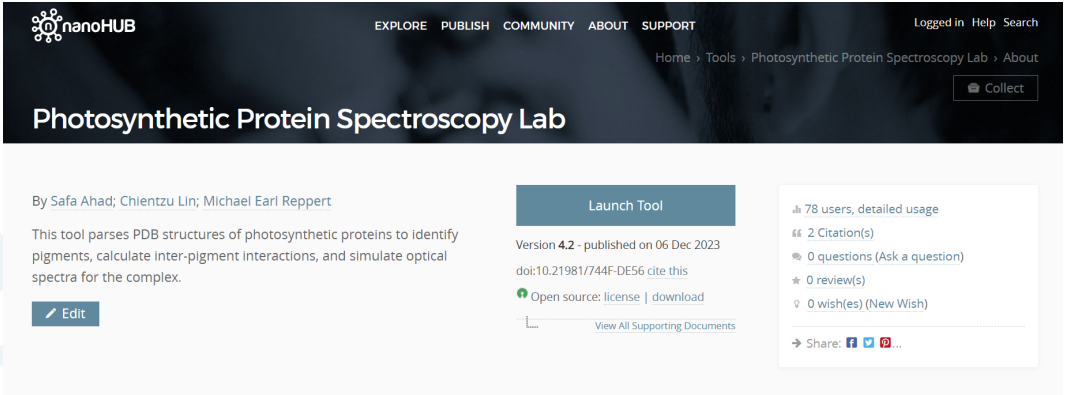
PigmentHunter: The 'Point-and-Click' Simulation Tool



We designed an *accessible* and *efficient* computational tool, PigmentHunter, that automates *predicting optical spectra* from *protein structure* of photosynthetic pigment complexes.(Srivastava et al. 2021)

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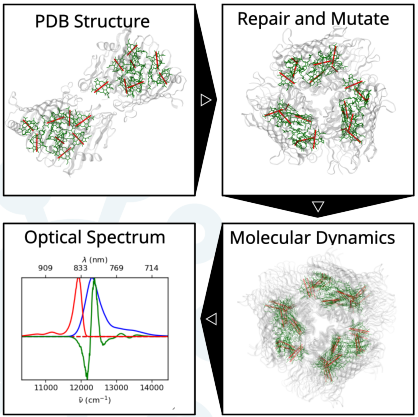
An Overview of PigmentHunter's Workflow



1. Identify, classify, and visualize pigments
2. Repair errors (e.g., missing atoms) in pigment and protein structures with biosymmetry
3. Prepare and run MD simulations and trajectories
4. Calculate optical spectra using the Frenkel exciton model

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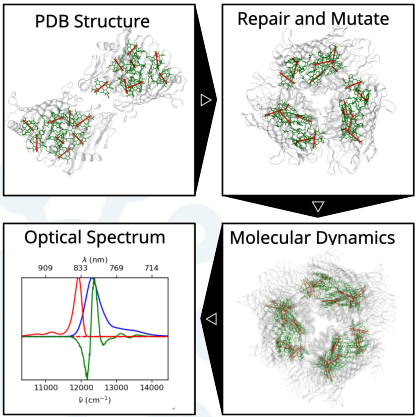

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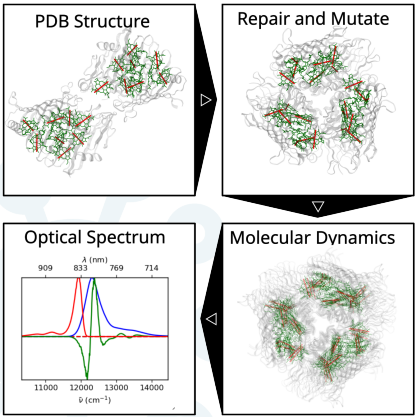

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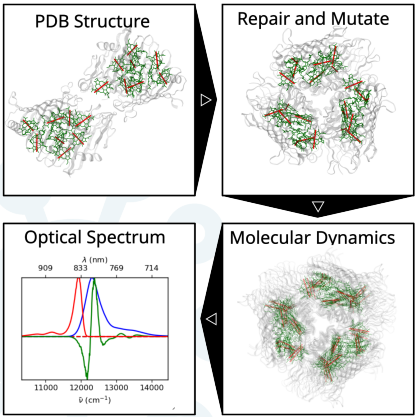

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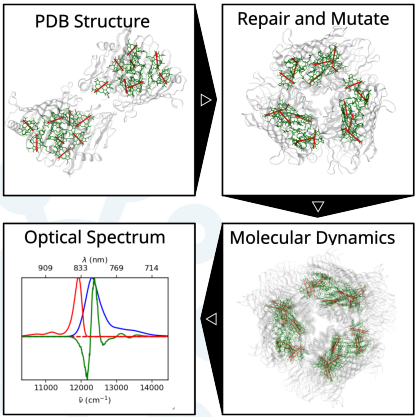

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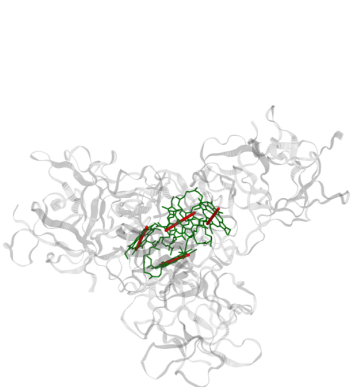
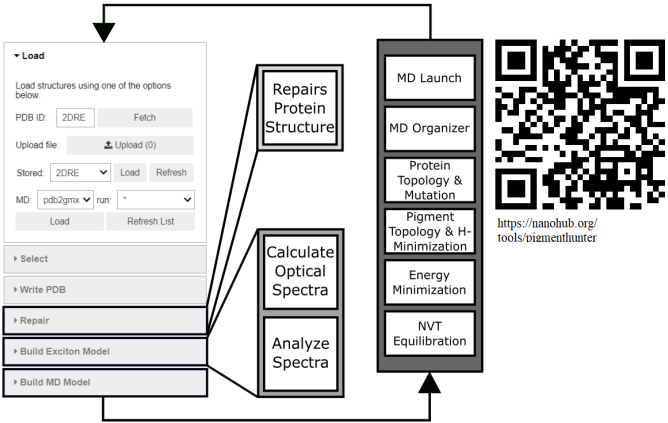
Main Window

1. Characterizing Pigments





https://nanohub.org/tools/pigmenthunter

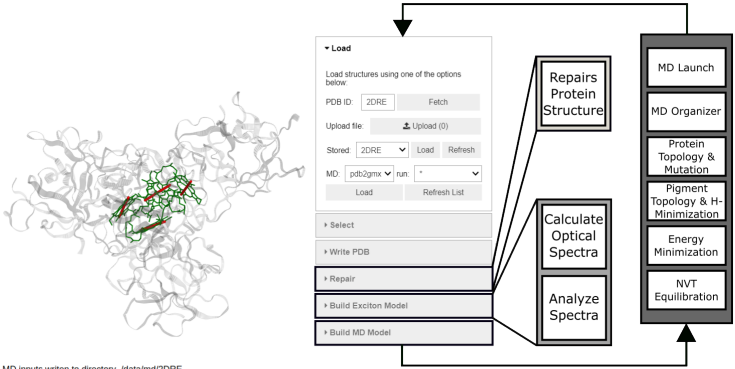
MD inputs writen to directory ./data/md/2DRE.

- Pigment List
- Automated Processing
- Code Entry

nanoHub Embedded Libraries

1. Characterizing Pigments

- ipywidgets
- NGLView
- HubLib
- Parmed
- gromacs-2018.4



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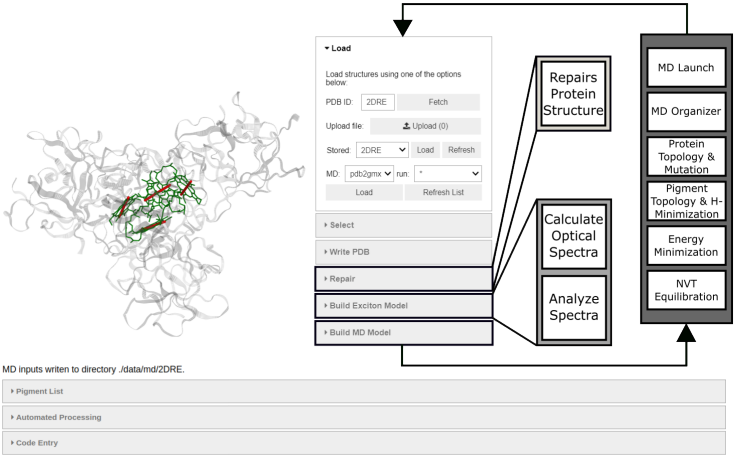


FloatText

```
widgets.FloatText(
    value=7.5,
    description='Any:',
    disabled=False
)
```

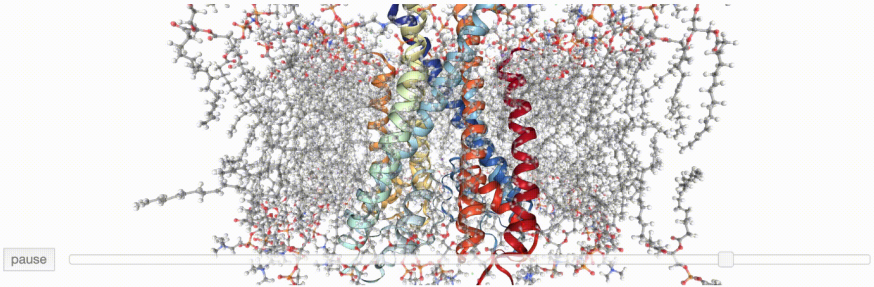
Any: 7.5

NGLView

1. Characterizing Pigments

In [1]:
```
import pytraj as pt
import nglview as nv
```

In [2]:
```
traj =  pt.load('sim.nc', top='sim.prmtop')
view = nv.show_pytraj(traj)
view
```



In [3]:
```
view.clear()
view.add_cartoon('protein', color_scheme='residueindex')
view.add_ball_and_stick('not protein', opacity=0.5)
```

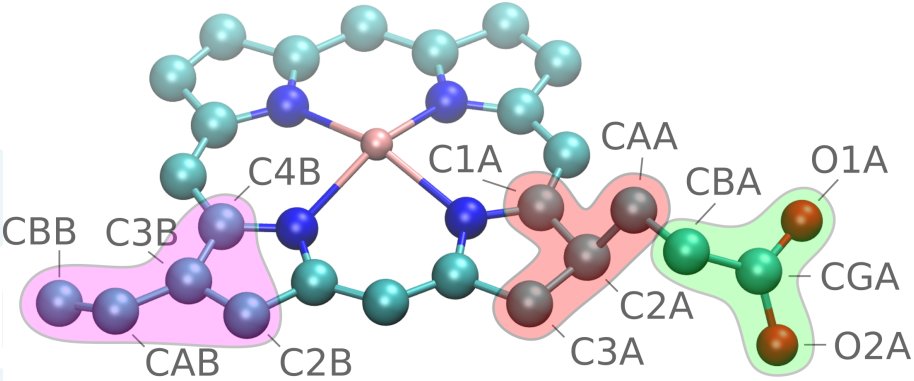
Pigments

Pigment	Code	μ_{eff}	PDC	TrEsp	NSD	MD	CDC
Chl *a*	CLA	4.3 D	Y	Y	Y	Y	Y
Pheo *a*	PHA	3.5 D	Y	Y	Y*	N	N‡
Chl *b*	CLB	3.6 D	Y	Y	Y	N	N‡
BChl *a*	BCA	5.45 D	Y	Y	Y†	Y	Y

- * = used NSD parameters from CLA
- † = NSD coefficients available only
- ‡ = CDC parameters installed but cannot use without MD

Pigment Repairs and Biosymmetry Operations

2. Repairs and Mutations



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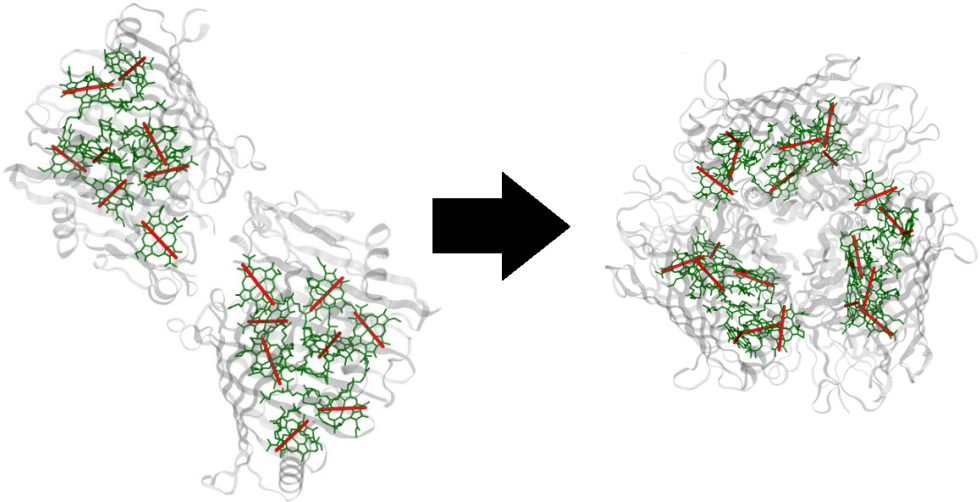
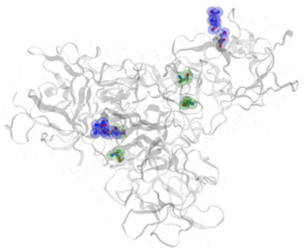


Protein Repairs and Mutations

2. Repairs and Mutations

https://nanohub.org/tools/PigmentHunter



Mutate Residue: D/GLN 57 (D to: ALA Mutate

Mutations: A/GLN 57 (A:55) to ALA
B/GLN 57 (B:375) to ALA
C/GLN 57 (C:705) to ALA
D/GLN 57 (D:1021) to ALA
Remove

Build Topology

A/GLN 57 (A:55) to ...
B/GLN 57 (B:375) t...
C/GLN 57 (C:705) t...
D/GLN 57 (D:1021)...
161--162
457--458

Round 1: Res 161 -- 162 long bond: Chain break

Warning: Long Bond (2406-2408 = 1.01839 nm)

Bond between atoms 1214 and 1220 was long (10.18).
Identified atoms as belonging to residues 161 and 162
Inserting chain break between them.

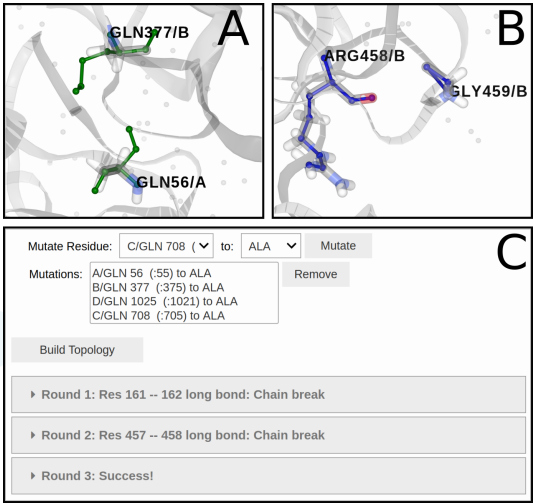
Checking for duplicate atoms....
Generating any missing hydrogen atoms and/or adding termini.
Now there are 177 residues with 2654 atoms
Chain time...
Processing chain 4 'D' (1353 atoms, 177 residues)
Identified residue ASP968 as a starting terminus.
Identified residue ASP1144 as a ending terminus.
Start terminus ASP-968: NH3+
End terminus ASP-1144: COO-
Checking for duplicate atoms....
Generating any missing hydrogen atoms and/or adding termini.
Now there are 177 residues with 2654 atoms
Chain time...
Processing chain 5 (150 atoms, 150 residues)
Problem with chain definition, or missing terminal residues.
This chain does not appear to contain a recognized chain molecule.
If this is incorrect, you can edit residuetypes.dat to modify the behavior.
Checking for duplicate atoms....
Generating any missing hydrogen atoms and/or adding termini.

Round 2: Res 457 -- 458 long bond: Chain break

Round 3: Success!

Protein Repairs and Mutations

2. Repairs and Mutations



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Click the buttons on the left to launch each step in the MD initialization process. Checking the checkbox to the right of each button will enable you to launch the next step.

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Build Pigment Topology	☑ Validate
Minimize Energy	☑ Validate
Run NVT	☐ Validate

All MD jobs are run using the standby queue on the HPC Negishi.

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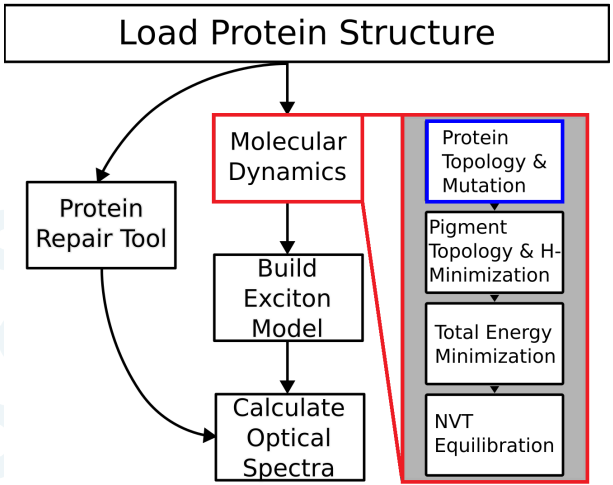
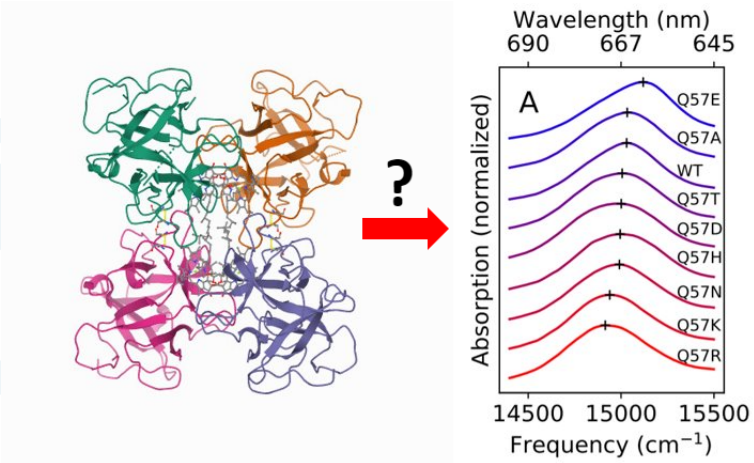
PyMol and Gromacs Implementation

3. Molecular Dynamics and Trajectories



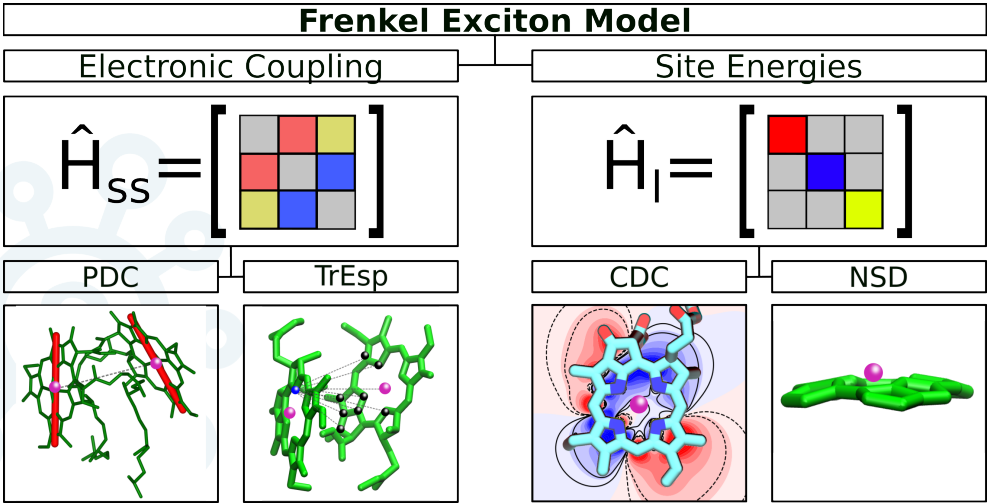
Structure-Spectrum Connection

4. Optical Spectrum from Exciton Modelling



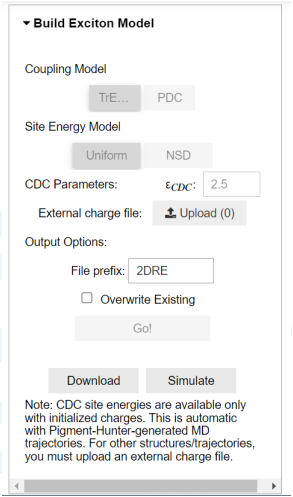
The Frenkel Exciton Model

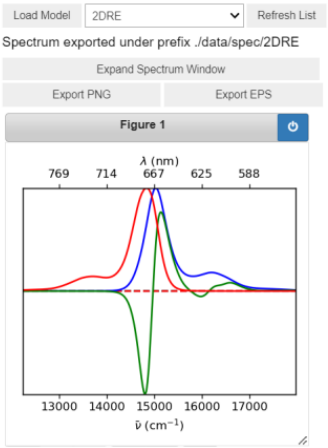
4. Optical Spectrum from Exciton Modelling

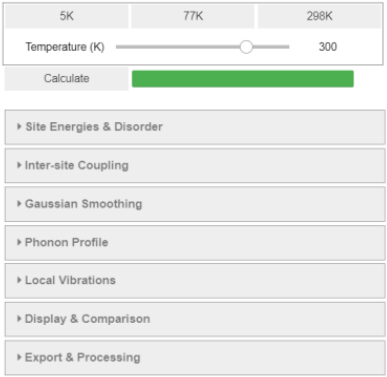


Exciton Menu and Spectrum Calculation Window

4. Optical Spectrum from Exciton Modelling







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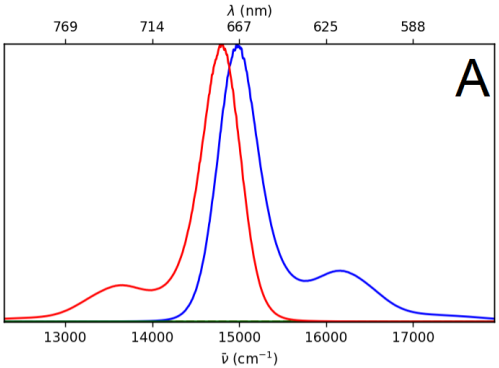
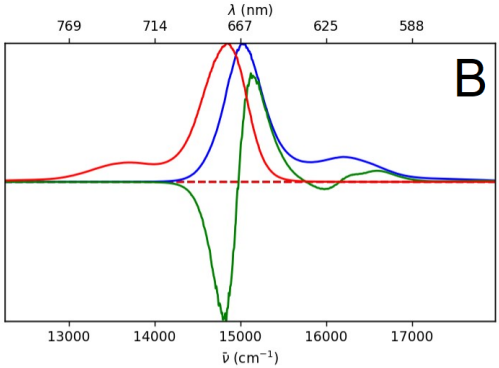
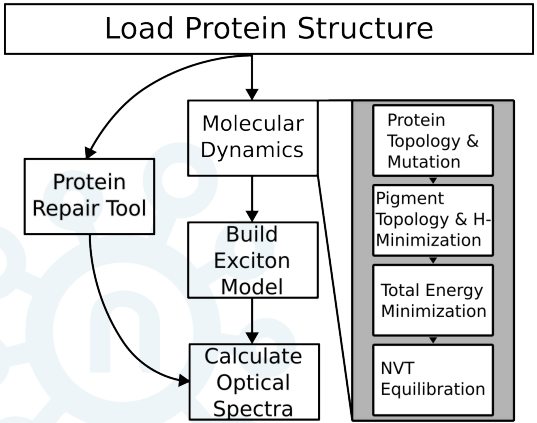
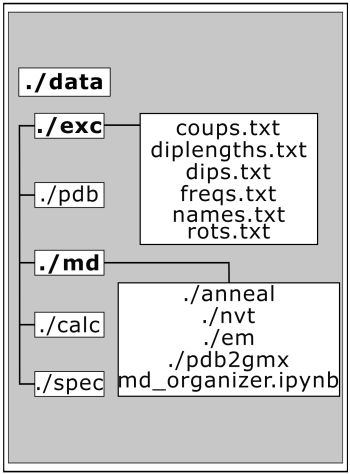




Brief Overview and File Organization





Predicting Experimental Electrostatic Frequency Shifts

Accurate prediction of mutation-induced frequency shifts in chlorophyll proteins with a simple electrostatic model

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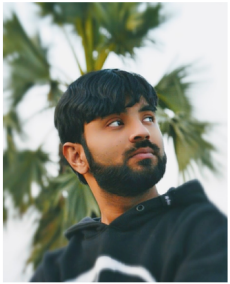
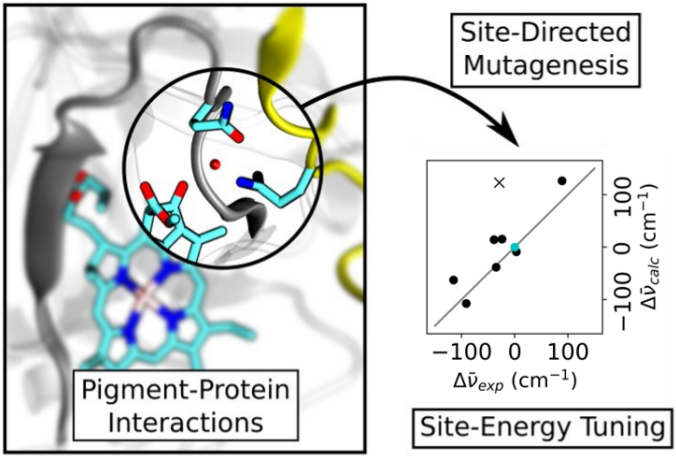


Dr. Amit Srivastava
Postdoctoral Researcher

Predicting Experimental Electrostatic Frequency Shifts



Experimental absorption shifts for eight water-soluble chlorophyll protein point mutants at the glutamine 57 site were compared with PigmentHunter.

Ring Distortion Site Energies with PSI and PSII

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Feeling the Strain: Quantifying Ligand Deformation in Photosynthesis

Chientzu Lin, Yuval Mazor, and Mike Reppert*

Cite this: *J. Phys. Chem. B* 2024, 128, 10, 2266–2280
Publication Date: March 5, 2024
https://doi.org/10.1021/acs.jpcb.3c06488

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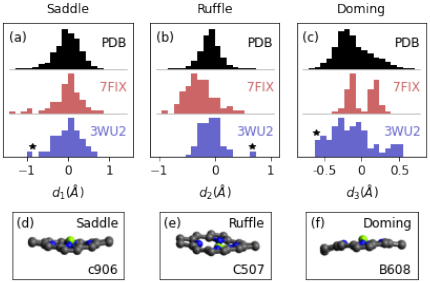
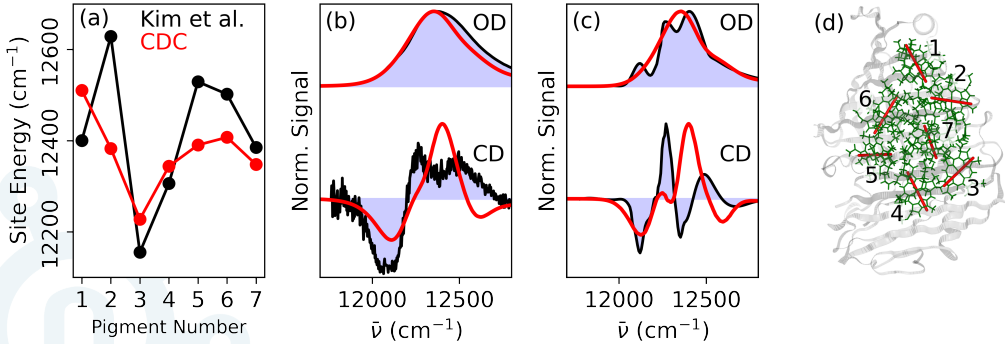
Ring Distortion Site Energies with PSI and PSII



PSI, shown in red, and PSII, blue, structure site energies are shown with the black stars marking deformation values for each structure.

Site Energy Calculations for Low Symmetry FMO Complex



The Fenna-Matthews-Olson (FMO) protein is a more complex model to compare how the charge density coupling (CDC) model compares to electronic structure site energy calculation data from Kim et al. 2020.

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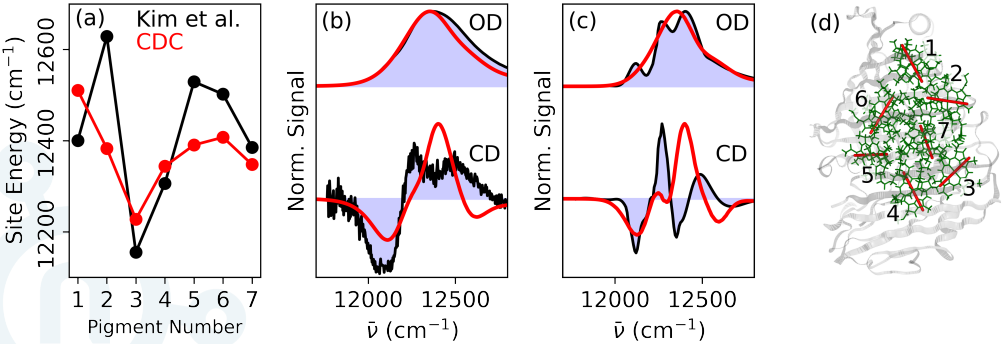
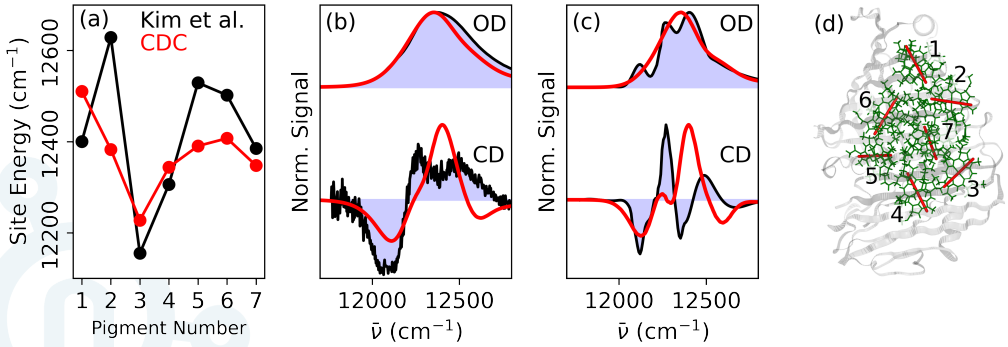


- PigmentHunter CDC vs QM/MM site energies

Site Energy Calculations for Low Symmetry FMO Complex



- PigmentHunter's absorption and CD spectra vs. corresponding experimental spectra at 295K

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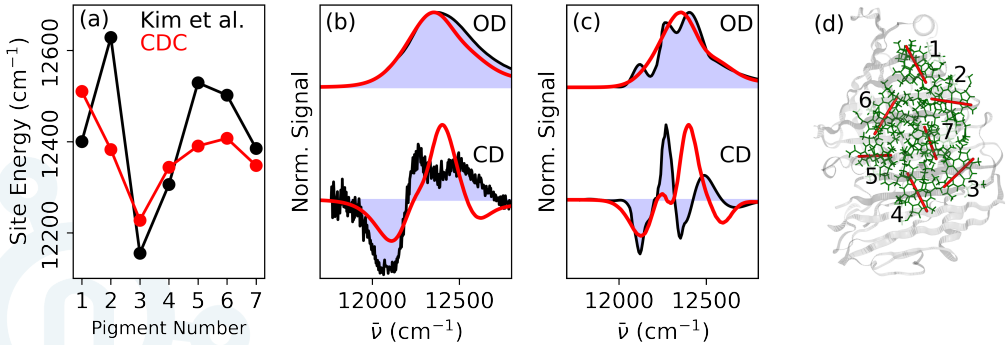
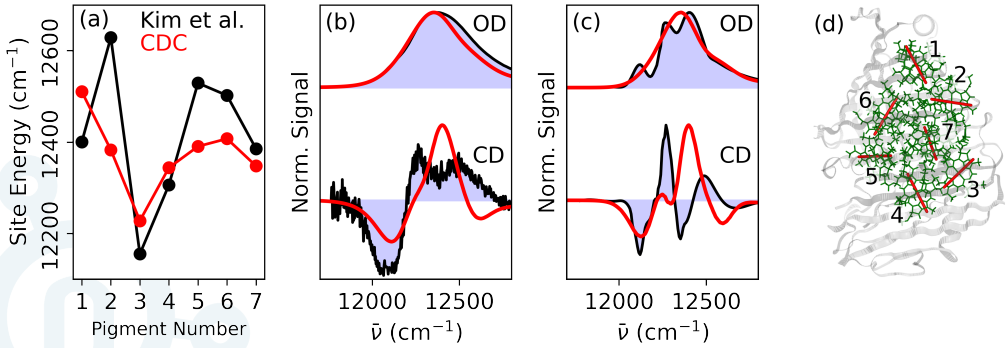


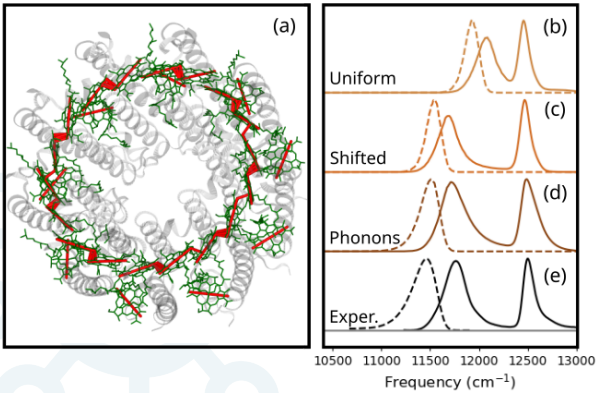
- PigmentHunter's absorption and CD spectra vs. corresponding experimental spectra at 77K

Site Energy Calculations for Low Symmetry FMO Complex



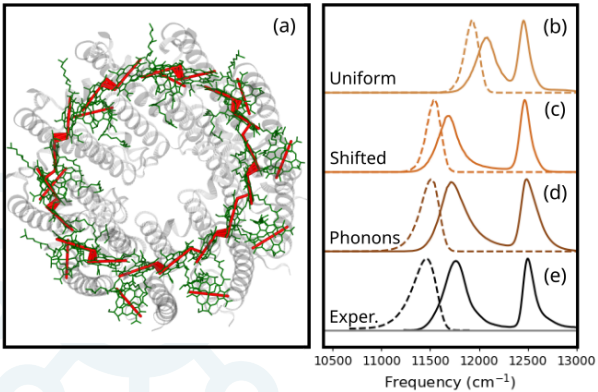
- Site numbering where 8th site is excluded from PigmentHunter calculations

Adjusting Excitonic Parameters with LH2



- Temperature at 5K and TrEsp couplings
- Gaussian Disorder, FWHM, 500 cm^{-1} B850 ring and 145 cm^{-1} for the B800 ring.
- **Uniform Site Energies:** 12500 cm^{-1}
- **Shifted Site Energies:** for the B850 and B800 rings to 12110 cm^{-1} and 12510 cm^{-1}.
- **Phonons:** S $= 0.8$

Adjusting Excitonic Parameters with LH2



- Temperature at 5K and TrEsp couplings
- Gaussian Disorder, FWHM, 500 cm^{-1} B850 ring and 145 cm^{-1} for the B800 ring.
- **Uniform Site Energies:** 12500 cm^{-1}
- **Shifted Site Energies:** for the B850 and B800 rings to 12110 cm^{-1} and 12510 cm^{-1}.
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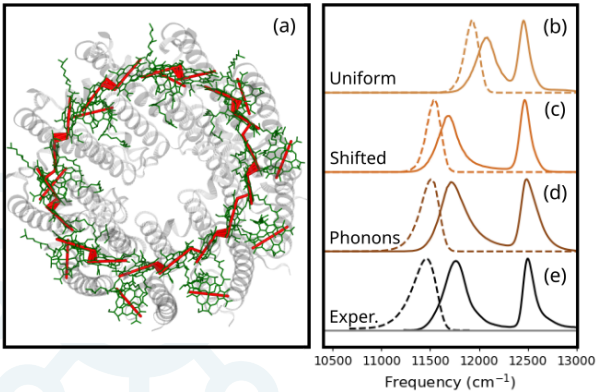

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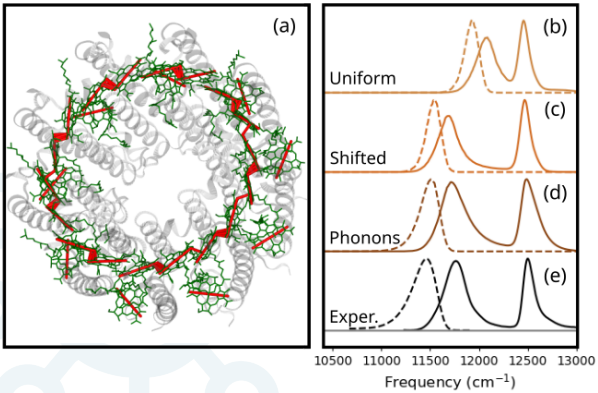

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Conclusions

With PigmentHunter we have demonstrated how to utilize nanoHUB's capabilities to create:

- User friendly graphically interface
- Automate molecular dynamics
- Automate Optical Spectrum Prediction

Paper coming soon.