

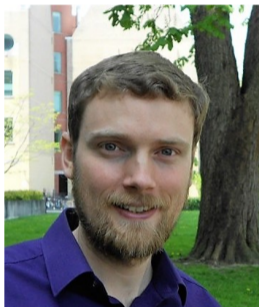
Building a nanoHUB Graphical Interface for Exploring Protein Dynamics and Spectroscopy: the PigmentHunter App.

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



Reppert Group, Purdue University
April 4th 2024

Acknowledgements



Dr. Mike Reppert
Assistant Professor



Chientzu Lin
Undergraduate
Researcher

- nanoHUB (host)
- ITaP
- Dr. Danilo Roccatano (GROMACS force fields for chlorophyll)
- Dr. Thomas Renger (transition partial charges)
- U.S. Department of Energy, Award/Contract Number DE-SC0022884

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

1 Background and Significance

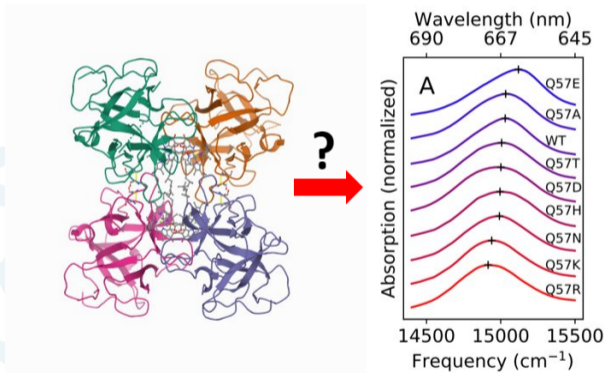
2 PigmentHunter Interface and Workflow

3 Applications and Examples



Motivation

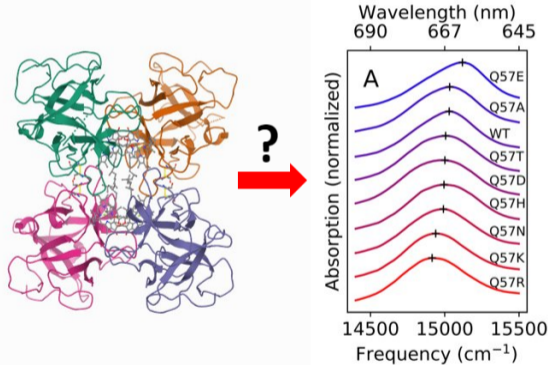
Understanding the connection between protein-pigment complex structure and optical function is complicated, making it difficult to design PPCs.



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

Motivation

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



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

Checklist:

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

Checklist:

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

Checklist:

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

Checklist:

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

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

nanoHUB

EXPLORE PUBLISH COMMUNITY ABOUT SUPPORT

Logged in Help Search

Home > Tools > Photosynthetic Protein Spectroscopy Lab > About

Collect

Photosynthetic Protein Spectroscopy Lab

By [Safa Ahad](#); [Chientzu Lin](#); [Michael Earl Reppert](#)

This tool parses PDB structures of photosynthetic proteins to identify pigments, calculate inter-pigment interactions, and simulate optical spectra for the complex.

Edit

Launch Tool

Version **4.2** - published on 06 Dec 2023
doi:10.21981/744F-DE56 [cite this](#)

Open source: [license](#) | [download](#)

View All Supporting Documents

- 78 users, [detailed usage](#)
- 2 [Citation\(s\)](#)
- 0 questions ([Ask a question](#))
- 0 review(s)
- 0 wish(es) ([New Wish](#))

→ Share: ...

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)

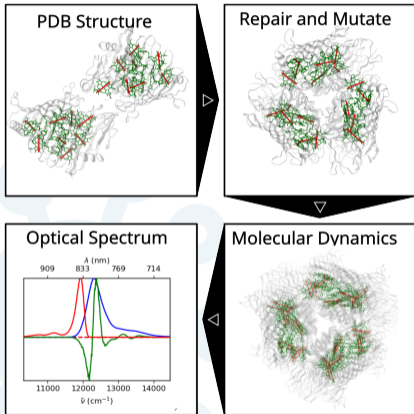
1 Background and Significance

2 PigmentHunter Interface and Workflow

- Characterizing Pigments
- Repairs and Mutations
- Molecular Dynamics and Trajectories
- Optical Spectrum from Exciton Modelling

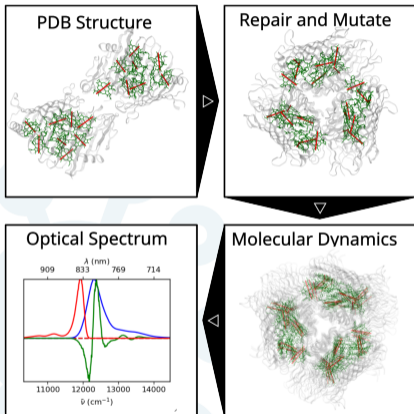
3 Applications and Examples

An Overview of PigmentHunter's Workflow



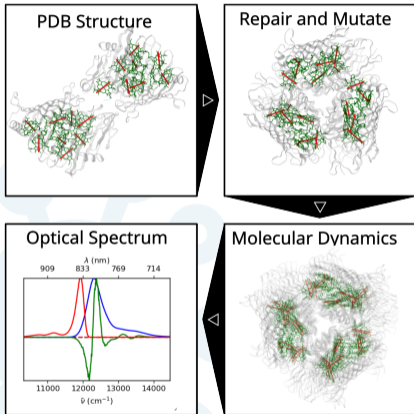
- 1 Identify, classify, and visualize pigments
- 2 Repair errors (e.g., missing atoms) in pigment and protein structures with biosymmetry
- 3 Prepare and run MD simulations and trajectories
- 4 Calculate optical spectra using the Frenkel exciton model

An Overview of PigmentHunter's Workflow



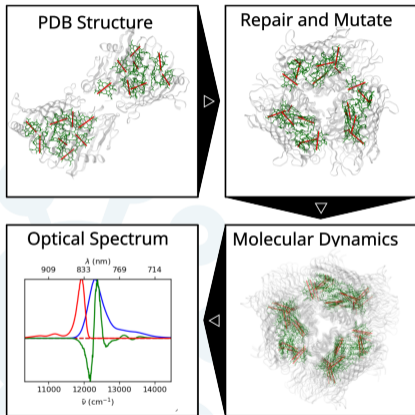
- 1 Identify, classify, and visualize pigments
- 2 Repair errors (e.g., missing atoms) in pigment and protein structures with biosymmetry
- 3 Prepare and run MD simulations and trajectories
- 4 Calculate optical spectra using the Frenkel exciton model

An Overview of PigmentHunter's Workflow



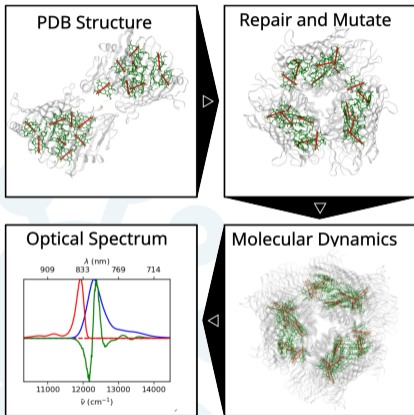
- 1 Identify, classify, and visualize pigments
- 2 Repair errors (e.g., missing atoms) in pigment and protein structures with biosymmetry
- 3 Prepare and run MD simulations and trajectories
- 4 Calculate optical spectra using the Frenkel exciton model

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

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

1 Background and Significance

2 PigmentHunter Interface and Workflow

- Characterizing Pigments

- Repairs and Mutations

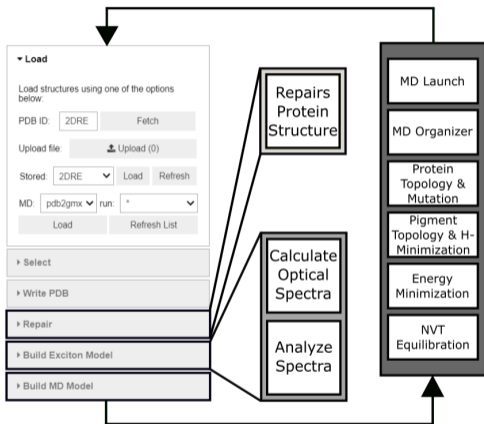
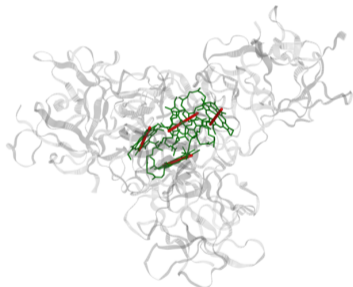
- Molecular Dynamics and Trajectories

- Optical Spectrum from Exciton Modelling

3 Applications and Examples

Main Window

1. Characterizing Pigments



<https://nanohub.org/tools/pigmenthunter>

MD inputs written to directory `./data/md/2DRE`.

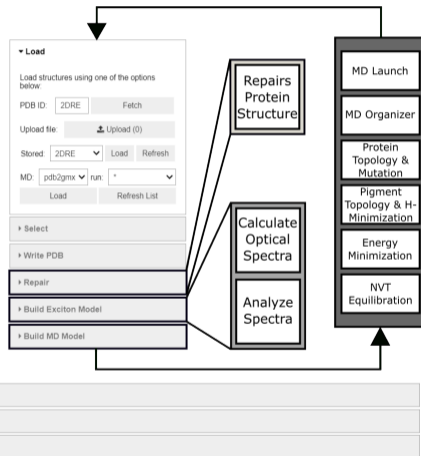
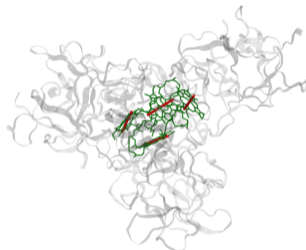
▶ Pigment List
▶ Automated Processing
▶ Code Entry



nanoHub Embedded Libraries

1. Characterizing Pigments

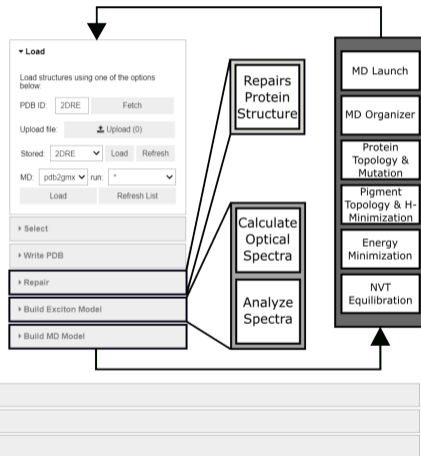
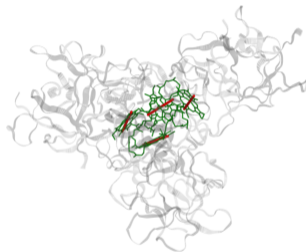
- ipywidgets
- NGLView
- HubLib
- Parmed
- gromacs-2018.4



nanoHub Embedded Libraries

1. Characterizing Pigments

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



iPywidgets

1. Characterizing Pigments

FloatText

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

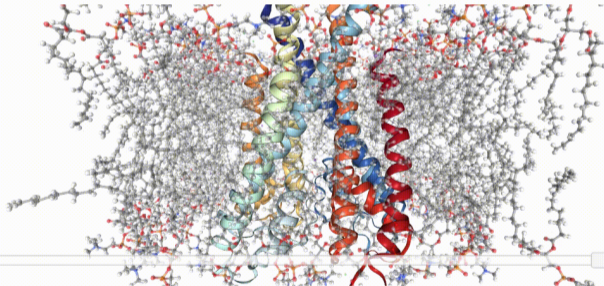
Any:

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

1. Characterizing Pigments

Pigment	Code	μ_{eff}	PDC	TrEsp	NSD	MD	CDC
Chl <i>a</i>	CLA	4.3 D	Y	Y	Y	Y	Y
Pheo <i>a</i>	PHA	3.5 D	Y	Y	Y*	N	N [‡]
Chl <i>b</i>	CLB	3.6 D	Y	Y	Y	N	N [‡]
BChl <i>a</i>	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

1 Background and Significance

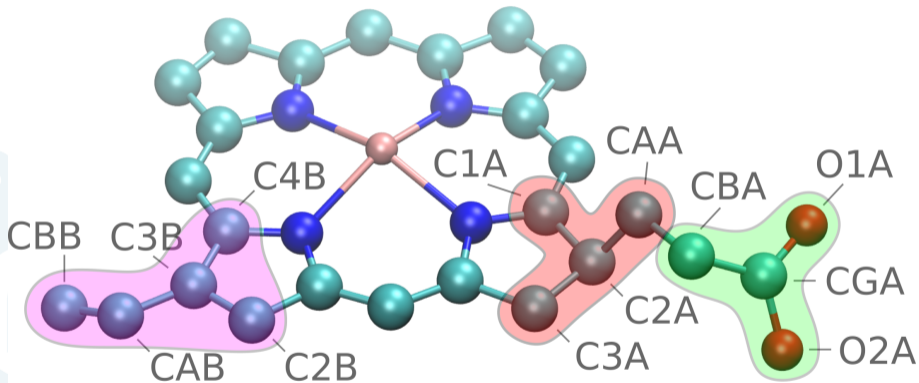
2 PigmentHunter Interface and Workflow

- Characterizing Pigments
- **Repairs and Mutations**
- Molecular Dynamics and Trajectories
- Optical Spectrum from Exciton Modelling

3 Applications and Examples

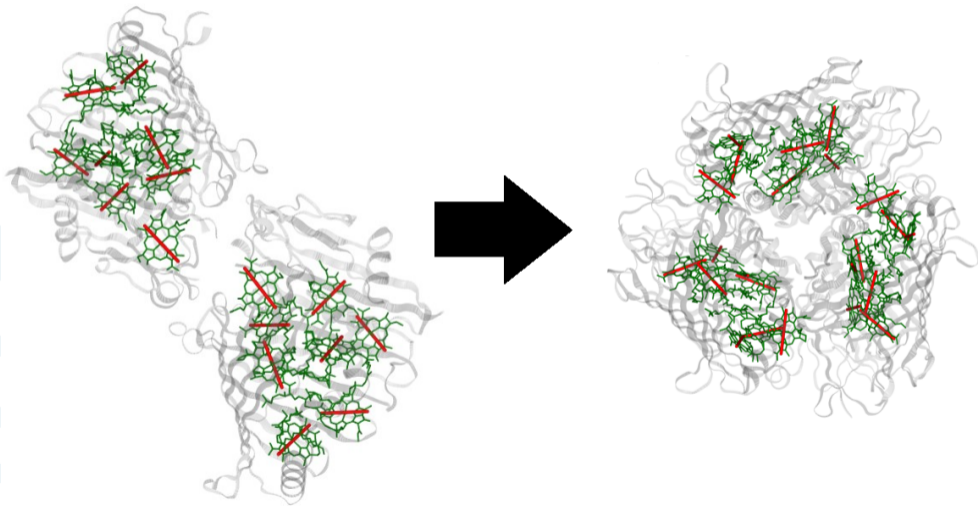
Pigment Repairs and Biosymmetry Operations

2. Repairs and Mutations



Pigment Repairs and Biosymmetry Operations

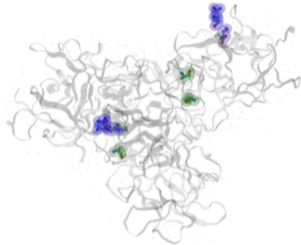
2. Repairs and Mutations



Protein Repairs and Mutations

2. Repairs and Mutations

<https://nanohub.org/tools/PigmentHunter>



Mutate Residue: D/GLN 57 (C) 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 an 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...

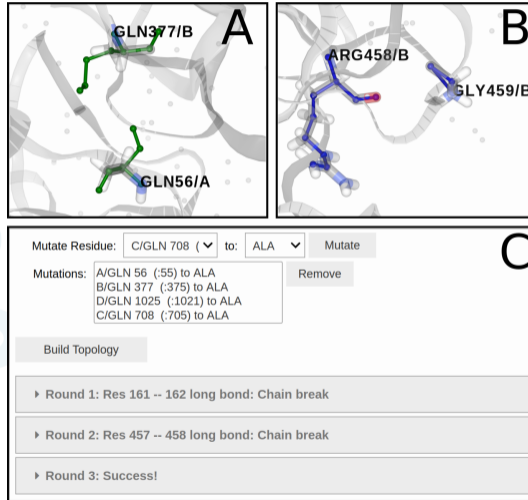
Generating any missing hydrogen atoms and/or adding termini.

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

Round 3: Success!

Protein Repairs and Mutations

2. Repairs and Mutations



The screenshot displays the PigmentHunter interface, divided into three main sections: A, B, and C.

Section A: Shows a protein structure with two highlighted residues: **GLN377/B** (top) and **GLN56/A** (bottom), both shown in green sticks.

Section B: Shows a protein structure with two highlighted residues: **ARG458/B** (left) and **GLY459/B** (right), both shown in blue sticks.

Section C: Shows the mutation control interface. At the top, it says "Mutate Residue: C/GLN 708 (v) to: ALA (v) Mutate". Below this, a list of mutations is shown: "Mutations: A/GLN 56 (:55) to ALA, B/GLN 377 (:375) to ALA, D/GLN 1025 (:1021) to ALA, C/GLN 708 (:705) to ALA". A "Remove" button is next to the list. Below the mutations is a "Build Topology" button. At the bottom, a log shows the repair progress: "Round 1: Res 161 -- 162 long bond: Chain break", "Round 2: Res 457 -- 458 long bond: Chain break", and "Round 3: Success!".

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

Molecular Dynamics (MD) Organizer

3. Molecular Dynamics and Trajectories

1 MD Organizer

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.

Don't click the checkbox until you've reviewed the output from the previous step and confirmed that it is correct!

Build Protein Topology

Validate

Build Pigment Topology

Validate

Minimize Energy

Validate

Run NVT

Validate

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

Molecular Dynamics (MD) Organizer

3. Molecular Dynamics and Trajectories

1 MD Organizer

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.

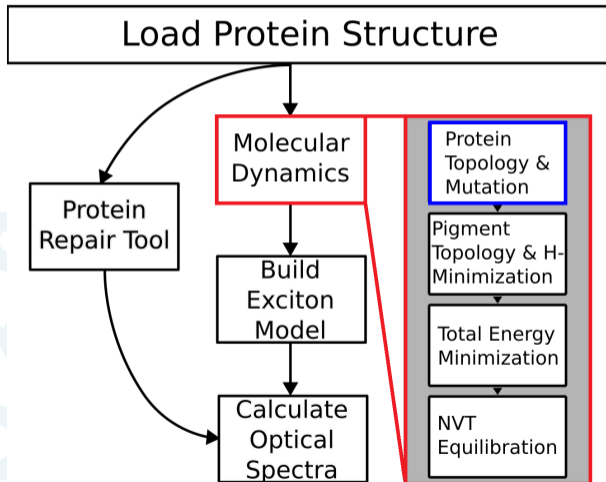
Don't click the checkbox until you've reviewed the output from the previous step and confirmed that it is correct!

Build Protein Topology	<input checked="" type="checkbox"/> Validate
Build Pigment Topology	<input checked="" type="checkbox"/> Validate
Minimize Energy	<input checked="" type="checkbox"/> Validate
Run NVT	<input type="checkbox"/> Validate

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

PyMol and Gromacs Implementation

3. Molecular Dynamics and Trajectories



1 Background and Significance

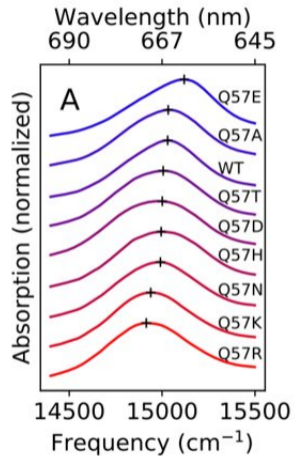
2 PigmentHunter Interface and Workflow

- Characterizing Pigments
- Repairs and Mutations
- Molecular Dynamics and Trajectories
- Optical Spectrum from Exciton Modelling

3 Applications and Examples

Structure-Spectrum Connection

4. Optical Spectrum from Exciton Modelling



The Frenkel Exciton Model

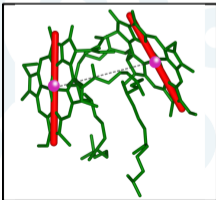
4. Optical Spectrum from Exciton Modelling

Frenkel Exciton Model

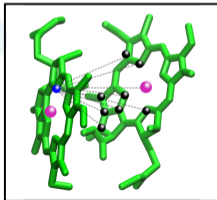
Electronic Coupling

$$\hat{H}_{SS} = \begin{bmatrix} \text{grey} & \text{red} & \text{yellow} \\ \text{red} & \text{grey} & \text{blue} \\ \text{yellow} & \text{blue} & \text{grey} \end{bmatrix}$$

PDC



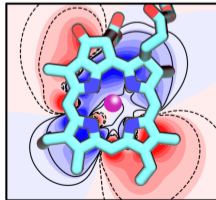
TrEsp



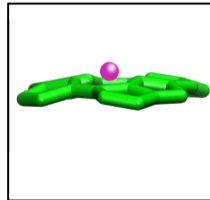
Site Energies

$$\hat{H}_I = \begin{bmatrix} \text{red} & \text{grey} & \text{grey} \\ \text{grey} & \text{blue} & \text{grey} \\ \text{grey} & \text{grey} & \text{yellow} \end{bmatrix}$$

CDC



NSD



Exciton Menu and Spectrum Calculation Window

4. Optical Spectrum from Exciton Modelling

▼ Build Exciton Model

Coupling Model
TrE... PDC

Site Energy Model
Uniform NSD

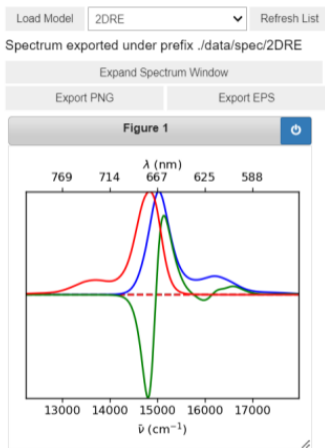
CDC Parameters: ϵ_{CDC} : 2.5

External charge file: Upload (0)

Output Options:
File prefix: 2DRE
 Overwrite Existing
Go!

Download Simulate

Note: CDC site energies are available only with initialized charges. This is automatic with Pigment-Hunter-generated MD trajectories. For other structures/trajectories, you must upload an external charge file.



5K 77K 298K

Temperature (K) 300

Calculate

► Site Energies & Disorder

► Inter-site Coupling

► Gaussian Smoothing

► Phonon Profile

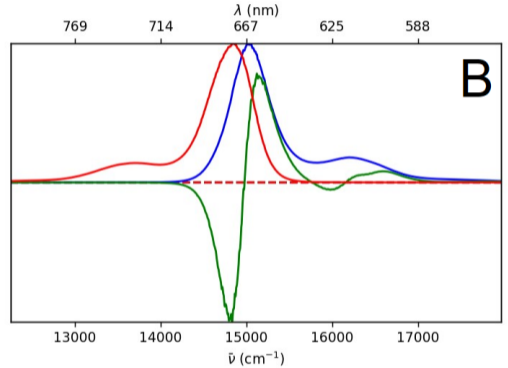
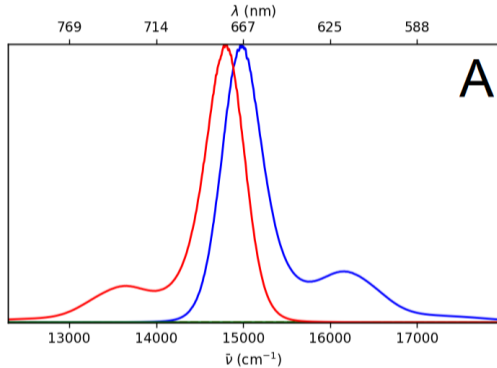
► Local Vibrations

► Display & Comparison

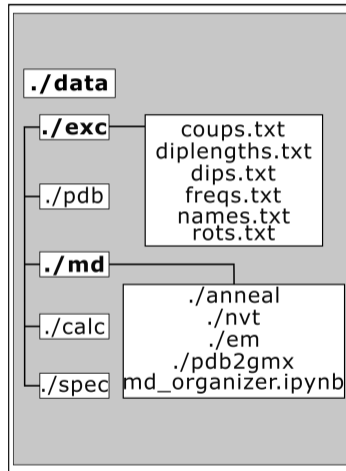
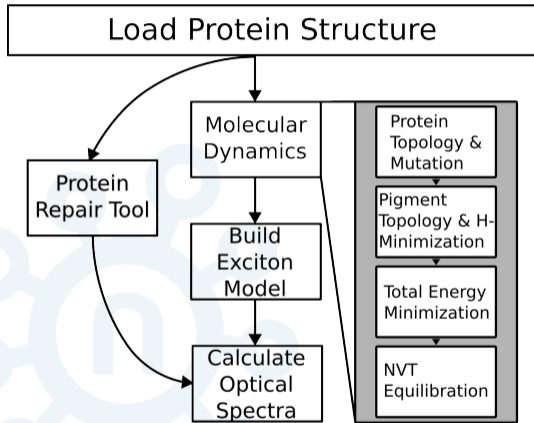
► Export & Processing

Exciton Menu and Spectrum Calculation Window

4. Optical Spectrum from Exciton Modelling



Brief Overview and File Organization



- 1 Background and Significance
- 2 PigmentHunter Interface and Workflow
- 3 Applications and Examples



Predicting Experimental Electrostatic Frequency Shifts

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

Cite as: *J. Chem. Phys.* **155**, 151102 (2021); doi: [10.1063/5.0064567](https://doi.org/10.1063/5.0064567)
Submitted: 24 July 2021 • Accepted: 30 September 2021 •
Published Online: 19 October 2021





View Online



Export Citation



CrossMark

Amit Srivastava, Safa Ahad,  Jacob H. Wat, and Mike Reppert^{*1} 

AFFILIATIONS

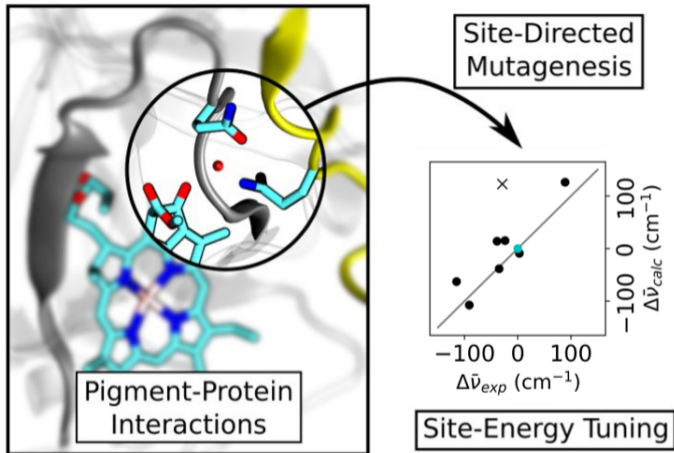
Department of Chemistry, Purdue University, West Lafayette, Indiana 47907, USA

^{*1}Author to whom correspondence should be addressed: reppertm@purdue.edu



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

RETURN TO ISSUE | < PREV **B: BIOPHYSICAL AND B...** NEXT >

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.jpcc.3c06488>

Copyright © 2024 American Chemical Society

[Request reuse permissions](#)

Article Views

114

Altmetric

1

Citations

-

[LEARN ABOUT THESE METRICS](#)

Share



Add to



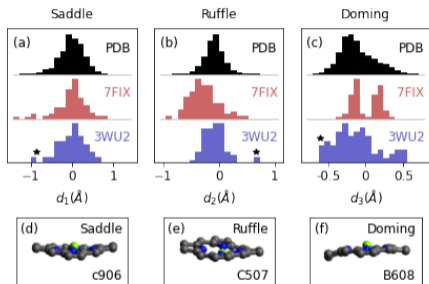
Export



Chientzu Lin
Undergraduate
Researcher

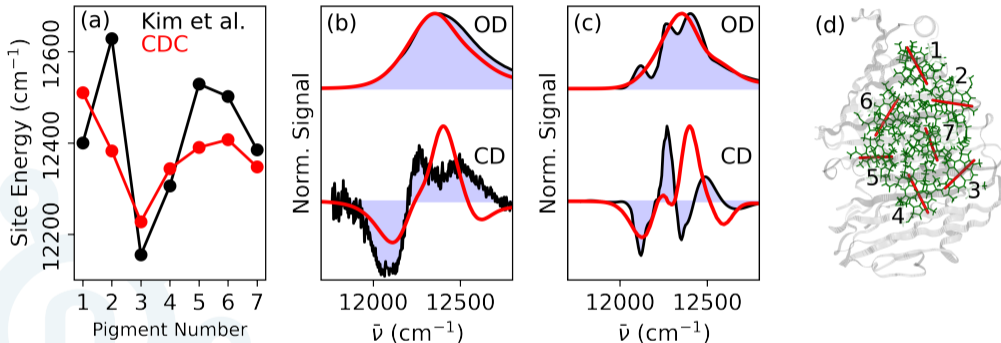


Ring Distortion Site Energies with PSI and PSII



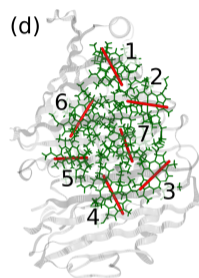
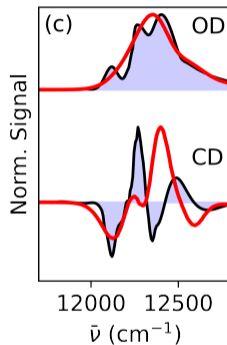
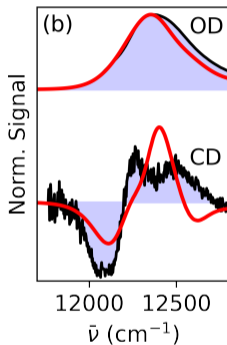
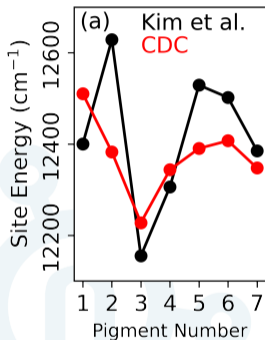
PSI, shown in red, and PSII, blue, structure site energies are shown with the black stars marking deformation values for each structure.

Site Energy Calculations for Low Symmetry FMO Complex



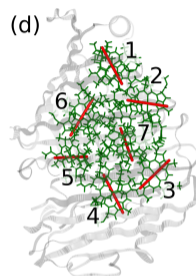
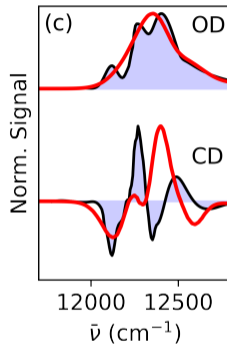
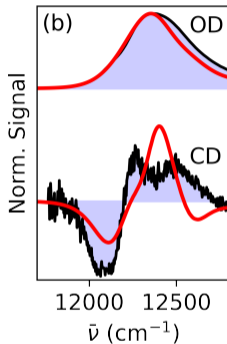
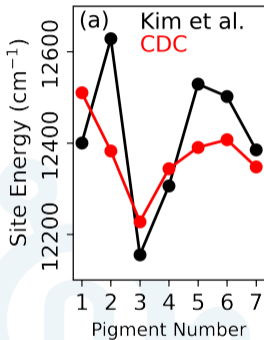
The Fenna-Matthews-Olson (FMO) protein is a more complex model to compare how the charge density coupling (CDC) model compares to electronic structure site energy calculation data from Kim et al. 2020.

Site Energy Calculations for Low Symmetry FMO Complex



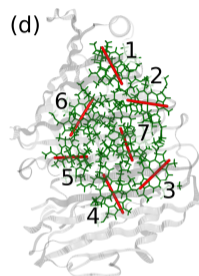
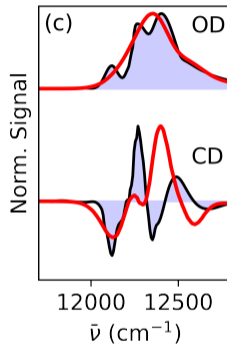
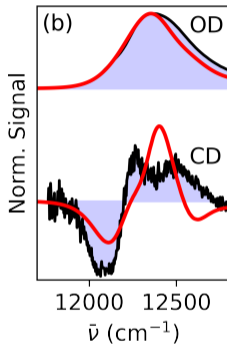
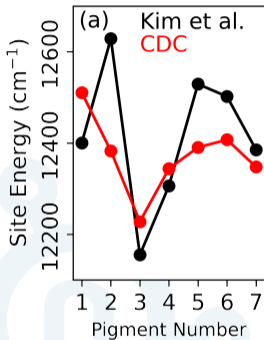
a PigmentHunter CDC vs QM/MM site energies

Site Energy Calculations for Low Symmetry FMO Complex



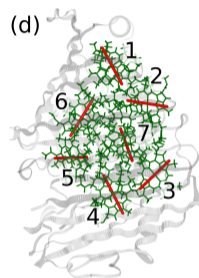
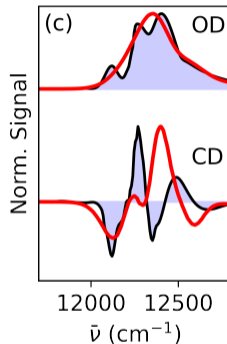
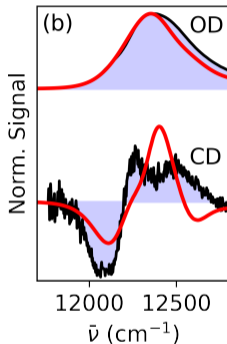
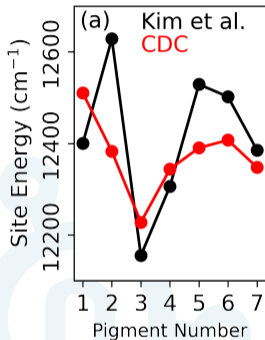
- b** PigmentHunter's absorption and CD spectra vs. corresponding experimental spectra at 295K

Site Energy Calculations for Low Symmetry FMO Complex



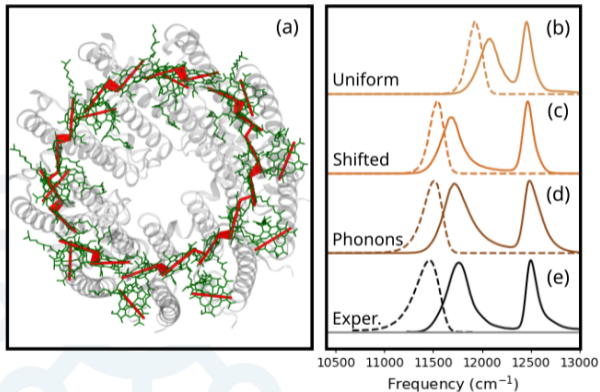
- c** PigmentHunter's absorption and CD spectra vs. corresponding experimental spectra at 77K

Site Energy Calculations for Low Symmetry FMO Complex



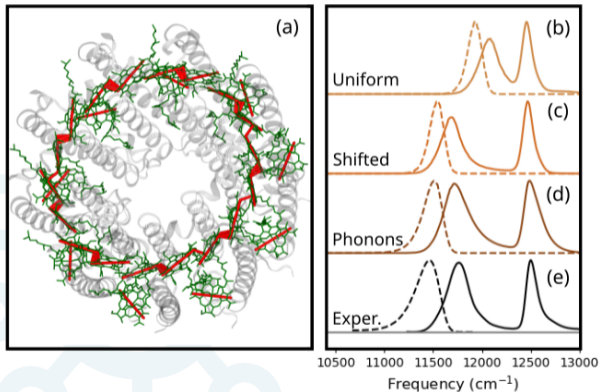
- d Site numbering where 8th site is excluded from PigmentHunter calculations

Adjusting Excitonic Parameters with LH2



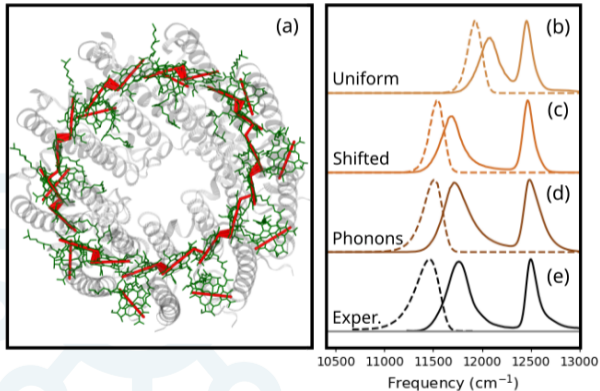
- Temperature at 5K and TrEsp couplings
- Gaussian Disorder, FWHM, 500 cm^{-1} B850 ring and 145 cm^{-1} for the B800 ring.
- Uniform Site Energies: 12500 cm^{-1}
- Shifted Site Energies: for the B850 and B800 rings to 12110 cm^{-1} and 12510 cm^{-1} .
- Phonons: $S = 0.8$

Adjusting Excitonic Parameters with LH2



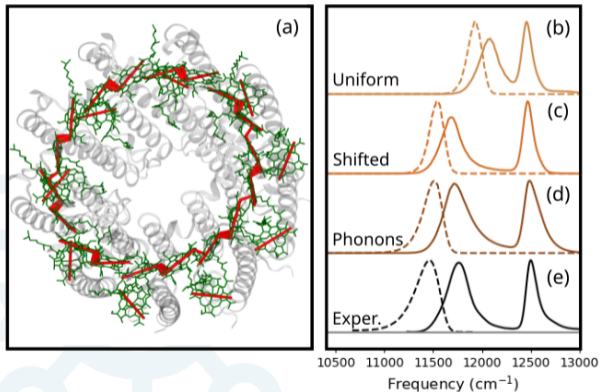
- Temperature at 5K and TrEsp couplings
- Gaussian Disorder, FWHM, 500 cm^{-1} B850 ring and 145 cm^{-1} for the B800 ring.
- **Uniform Site Energies:** 12500 cm^{-1}
- **Shifted Site Energies:** for the B850 and B800 rings to 12110 cm^{-1} and 12510 cm^{-1} .
- **Phonons:** $S = 0.8$

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} .
- **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} .
- **Phonons:** $S = 0.8$

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.

