## Project Status Report

# Project Summary

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| Report date | Project Name | Prepared By |
|  |  |  |

# Status Summary

Give a summary of project status here, including an overview of accomplishments from the last two weeks.

# Code and model development Tasks Self score \_\_\_\_\_ / 10 advisor score \_\_\_\_\_ / 10

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| --- | --- | --- | --- | --- |
| task | % Done | Due date | Purpose | outcomes |
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# Calculation/data collection/analysis tasks SElf score \_\_\_\_\_ / 10 advisor score \_\_\_\_ / 10

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| task | % done | due date | purpose | outcomes |
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# Reading / writing tasks SElf score \_\_\_\_\_ / 10 advisor score \_\_\_\_\_ / 10

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| Paper read / work written | purpose | outcomes |
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# most important action items for next two weeks

1. Optimize geometry of Eosin Y at RHF/6-311G level of theory, report total energy and HOMO/LUMO gap in eV
2. Optimize geometry of Eosin Y at RHF/cc-pVDZ level of theory, report energy and HOMO/LUMO gap in eV
3. Optimize geometry of Eosin Y at RHF/cc-pVTZ level of theory, report energy and HOMO/LUMO gap in eV
4. Optimize geometry of Eosin Y at B3LYP/6-311G level of theory, report energy and HOMO/LUMO gap in eV
5. Optimize geometry of Eosin Y at B3LYP/cc-pVDZ level of theory, report energy and HOMO/LUMO gap in eV
6. Optimize geometry of Eosin Y at B3LYP/cc-pVTZ level of theory, report energy and HOMO/LUMO gap in eV
7. Optimize geometry of Eoson Y at PBE0/6311G level of theory, report energy and HOMO/LUMO gap in eV
8. Optimize geometry of Eoson Y at PBE0/cc-pVDZ level of theory, report energy and HOMO/LUMO gap in eV
9. Optimize geometry of Eoson Y at PBE0/cc-pVTZ level of theory, report energy and HOMO/LUMO gap in eV
10. Using optimized geometry of B3LYP/cc-pVTZ calculation, find and report excitation energy using TDDFT at B3LYP/cc-pVTZ
11. Using optimized geometry of PBE0/cc-pVTZ calculation, find and report excitation energy using TDDFT at B3LYP/cc-pVTZ