**Experiment Project Documentation**

**Introduction**

This document captures the technical details related to the experiment development.

**Project**

**Domain Name:** Chemistry

**Lab Name:** Quantum Chemistry

**Experiment Name:** Geometric Optimization using ab initio calculations

**Purpose of the project**

# The purpose of this project is to convert experiment from Java3D to JavaScript Geometry Optimization using ab initio quantum calculations.

**Project Developers Details**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **S.NO** | **Names** | **Year of Study** | **Role** | **Email-ID** | **github handles** |
| 1. | Nishtala Venkata Sowmya | 4th year | . | Nishtala.sowmya@gmail.com | NishtalaSowmya |

**Technologies and Libraries**

**Technologies :**

1. HTML
2. CSS
3. Javascript

**Libraries :**

**THREE.js**

**Jquery**

**Development Environment**

**OS :** Windows 10

**Documents :**

|  |  |  |
| --- | --- | --- |
| **S.NO** | **Link to Document** | **Role** |
| 1. | Procedure | This document captures the instructions to run the simulations |
| 2. | Test Cases | This document captures the functional test cases of the experiment simulation |
| 3. | Code Documentation | This document captures the details related to code |

**Process Followed to convert the experiment**

1. Understand the assigned experiment Java simulation
2. Understanding the experiment concept
3. Re-implement the same in javascript

**Risks and Challenges**

1. Using THREE.js library

**Issues :**

No issues