Computational Molecular and Material Design Environment (CMMDE)

Background

This software is developed for decreasing the barrier in using popular open-source computational chemistry software. Currently, CMMDE can use the following software:

1. Orca
2. DFTB+
3. GROMACS
4. DOCK6
5. DCDFTBMD
6. Quantum Espresso
7. xTB via Orca
8. Open Babel

About CMMDE

CMMDE is a set of tools based on Python for running computational jobs, as well as analyzing, visualizing, and post-processing the results in free/libre and open source applications for computational molecular & material design.

- Core developers: Adit, Atthar, Hasan, MAM, Tommy
- Contributors: Athiya MH, Arifin, Daniel
- Core reviewers: Igun, Imam, Parsaoran
- Committed users: Yusthinus, Veli, Mirella, Riyanto, Badra, Hilda, Rustaman, Edu

Tahap kedua peluncuran CMMDE, didahului workshop:

15 Agustus 2022:
Workshop on Text-Based CMMDE

16 Agustus 2022:
Workshop on Web-Based CMMDE
Launching CMMDE: Web-Based Version
Launching Consortium on Computational Science Development
(Konsorsium Pengembangan Sains Komputasi)

Informasi lebih lanjut: cmmde@mki.or.id

Installation

1. Cloning the repository:

```
git clone https://git.mki.or.id/coredev/CMMDE
```

2. Change directory to CMMDE:

```
cd CMMDE
```

3. Install the code:

```
chmod +x install.sh
./install.sh
```