Python file of the optimized structure in the software：

PG

```
# Set up lattice
lattice = Triclinic(15.0*Angstrom, 3.637*Angstrom, 3.637*Angstrom,
90.0*Degrees, 90.0*Degrees, 90.0*Degrees)

# Define elements
elements = [Carbon, Carbon, Carbon, Carbon, Carbon, Carbon]

# Define coordinates
fractional_coordinates = [[ 0.540328,  0.435009,  0.934986],
                          [ 0.540328,  0.695356,  0.195334],
                          [ 0.5     ,  0.565184,  0.565162],
                          [ 0.5     ,  0.065184,  0.065162],
                          [ 0.459673,  0.195356,  0.434986],
                          [ 0.459673,  0.935009,  0.695334]]

# Set up configuration
bulk_configuration = BulkConfiguration(
    bravais_lattice=lattice,
    elements=elements,
    fractional_coordinates=fractional_coordinates
    )
```

POPG

```
# Set up lattice
lattice = BaseCenteredOrthorhombic(3.6833*Angstrom, 9.1124*Angstrom,
20.0*Angstrom)

# Define elements
elements = [Carbon, Carbon, Carbon, Carbon, Carbon, Carbon]

# Define coordinates
fractional_coordinates = [[ 0.577,  0.423,  0.5  ],
                          [ 0.423,  0.577,  0.5  ],
                          [ 0.016,  0.364,  0.5  ],
                          [ 0.364,  0.016,  0.5  ],
                          [ 0.984,  0.636,  0.5  ],
                          [ 0.636,  0.984,  0.5  ]]

# Set up configuration
bulk_configuration = BulkConfiguration(
    bravais_lattice=lattice,
    elements=elements,
    fractional_coordinates=fractional_coordinates
    )
```

ΘG

```
# Set up lattice
vector_a = [8.072431742642411, 0.0, 0.0]*Angstrom
vector_b = [5.486218161233725e-16, 8.959674193495534, 0.0]*Angstrom
vector_c = [8.206548021340282e-16, 8.206548021340282e-16,
13.40231]*Angstrom
lattice = UnitCell(vector_a, vector_b, vector_c)

# Define elements
elements = [Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
Carbon,
            Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
Carbon,
            Carbon, Carbon, Carbon, Carbon, Carbon, Carbon, Carbon,
Carbon,
            Carbon, Carbon, Carbon, Carbon]

# Define coordinates
fractional_coordinates = [[ 0.534283840542,  0.926243379652,
 0.499384068737],
                          [ 0.131837949589,  0.795862331485,
 0.499384068737],
                          [ 0.781766762691,  0.419134873039,
 0.499384068737],
                          [ 0.325118243692,  0.419134873039,
 0.499384068737],
                          [ 0.553442635711,  0.068045398005,
 0.499384068737],
                          [ 0.160121438777,  0.191511825485,
 0.499384068737],
                          [ 0.950423766509,  0.190303411491,
 0.499384068737],
                          [ 0.781766762691,  0.575153904618,
 0.499384068737],
                          [ 0.325118243692,  0.575153904618,
 0.499384068737],
                          [ 0.640176039648,  0.673234775099,
 0.499384068737],
                          [ 0.207210592289,  0.654720240197,
 0.499384068737],
```

```
                        [ 0.823651082161,  0.077514125265,
 0.499384068737],
                        [ 0.411851912668,  0.166126268486,
 0.499384068737],
                        [ 0.640176039648,  0.321054002558,
 0.499384068737],
                        [ 0.195982551348,  0.34759630306 ,
 0.499384068737],
                        [ 0.812950109879,  0.931954601995,
 0.499259113114],
                        [ 0.392693117498,  0.828162509171,
 0.499384068737],
                        [ 0.675874563585,  0.828162509171,
 0.499384068737],
                        [ 0.2317870005  ,  0.913936341104,
 0.499384068737],
                        [ 0.939171116874,  0.807128654697,
 0.499384068737],
                        [ 0.052293486704,  0.42347312513 ,
 0.498695211661],
                        [ 0.929987704074,  0.358651114986,
 0.499629721708],
                        [ 0.466708966735,  0.321054002558,
 0.499384068737],
                        [ 0.695033358755,  0.166126268486,
 0.499384068737],
                        [ 0.246649176753,  0.080909739808,
 0.499384068737],
                        [ 0.049576233491,  0.571134059722,
 0.501304788339],
                        [ 0.925491717691,  0.659650940996,
 0.500362575988],
                        [ 0.466708966735,  0.673234775099,
 0.499384068737]]

# Set up configuration
bulk_configuration = BulkConfiguration(
    bravais_lattice=lattice,
    elements=elements,
    fractional_coordinates=fractional_coordinates
    )
```