Converg King User Guide

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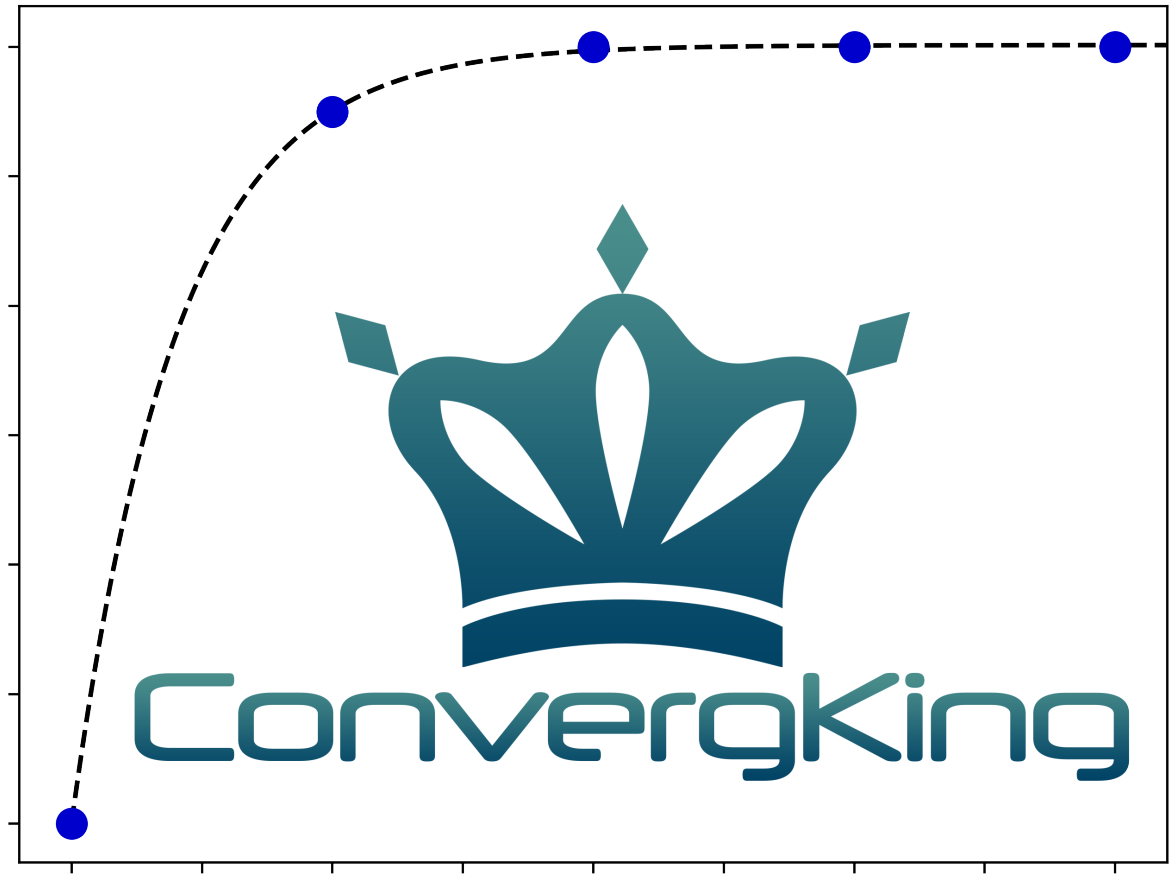

LEEDMOL
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1 Introduction

ConvergKing is a python script that automate the of electrostatic environment convergence for crystals as described at supermolecular method, Valverde et al. (2017).

2 Converg King - Input Files

ConvergKing make use of three input files:

A **info.in** file that contains the quantum-mechanics and crystal simmetry parameters, a info.in example is available on APP folder;
An example of info.in:

```
ncela = 18
nx = 7
ny = 7
nz = 7
name = acemid05
metodo = HF
base = 3-21g
mem = 10GB
cpu = 1
sheril = True
radii = Br 1.35
cMethod = ChelP
```

The description of keywords:

- **ncela** = this is a internal keyword to make the right replication. To get this number follow the equation below:

$$\textbf{ncela} = \frac{(nx * ny * nz * number\_of\_atoms\_in_a symmetric\_unit)}{len(supercell)} \tag{1}$$

$$\textbf{ncela} = \frac{(7 * 7 * 7 * 9)}{(55566)} \tag{2}$$

  The equation above it's for a crystal that has 9 atoms in they asymmetric unit and a supercell of 55566 atoms.

- **nx, ny and nz** are the number of times that was replicated in each direction;
- **name** is the name of the job;
- **metodo** is the quantum mechanics method that will be used. Examples: HF, B3LYP, MP2;
- **base** is the basis set that will be used;
- **mem** is the memory available for the job;
- **cpu** is the number of threads available for the job;
- **sheril** is **True** if the supercell was generated on Crystallate, Borca et al. (2019). If the supercell was generated in Mercury please set this keyword to **False**.
- **radii** is the van der Waals radii of the metal to put in .gjf file. (If not necessary just don't write this in info.in file)

- **cMethod** is the method that atomic partial charges will be calculated. Available: Chelp, ChelpG, CM5, Hirshfeld, MK, Mulliken, NBO, NPA, AIM. **OBS**: AIM requires *Multiwfn* software, Lu and Chen (2012). All the other methods will be calculated at *Gaussian 16* software Frisch et al. (2016).

A **assimetrical_unit.xyz** file that contain the atomic positioning of the asymmetrical unit;

A **supercell.xyz** file that contain the atomic positioning of the crystal lattice;

3 Converg King - Output Files

ConvergKing output file are:

- A dummy.gjf (Gaussian 16 input file) containing the converged charge field;
- The convergKing.out containing computational details of convergence process as well as the final converged ESP Charges;
- The dipole convergence graph.

4 Required libraries

ConvergKing requires the following libraries:

- *Moleking_util* [The authors would like to thank **Lopes TH** and **Mateus RB** for disponibilize the MoleKing_util chemical package.]
- Matplotlib;
- lmfit;
- os;
- sys;
- time;
- numpy;

5 Running Converg King

For running ConvergKing just type:

```
1    python3 PATH/ConvergKing/ConvergKing.py
```

Referências

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