Introduction of pygamess

RDKit UGM 2017

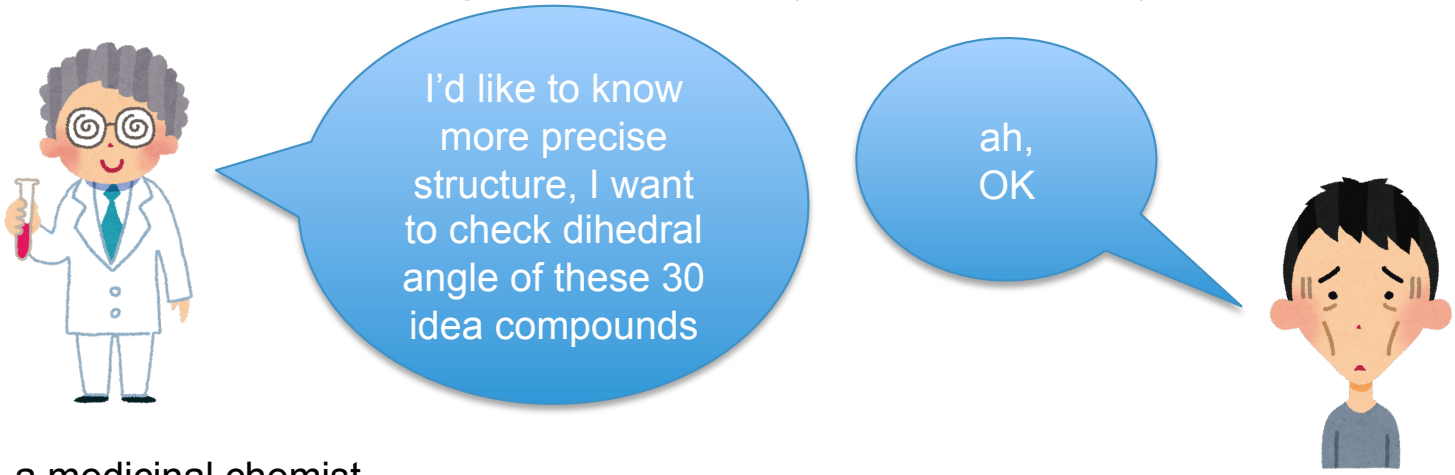
kazufumi ohkawa

Motivation

I’d like to add quantum chemical power to RDKit.

RDKit is very useful but ...

```
>>> from rdkit import Chem
>>> from rdkit.Chem import AllChem
>>> m = Chem.MolFromSmiles("CC")
>>> m = Chem.AddHs(m)
>>> AllChem.EmbedMolecule(m)
>>> AllChem.UFFOptimizeMolecule(m, maxIters=200)
```

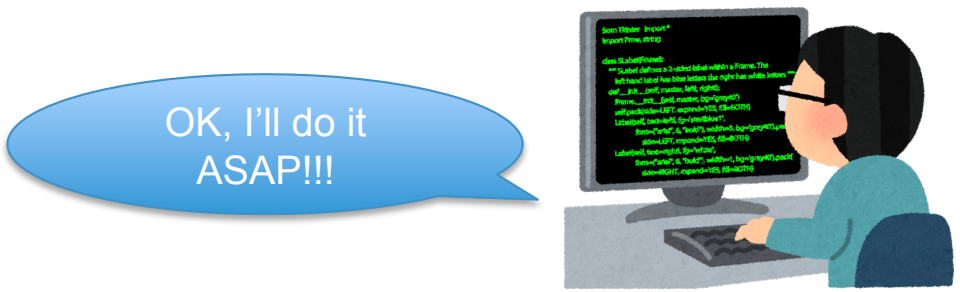


a medicinal chemist

me

If you... (It’s nice isn’t it?)

```
>>> from rdkit import Chem
>>> from rdkit.Chem import AllChem
>>> m = Chem.MolFromSmiles("CC")
>>> m = Chem.AddHs(m)
>>> AllChem.EmbedMolecule(m)
>>> AllChem.UFFOptimizeMolecule(m, maxIters=200)
>>> optimized_mol = QuantumChemicalOptimization(m)
>>> optimized_mol # return RDKit Chem object
```



Other situations quantum chemistry is needed

Photo toxicity prediction

HOMO-LUMO gap energy or Excited state affects photo toxicity

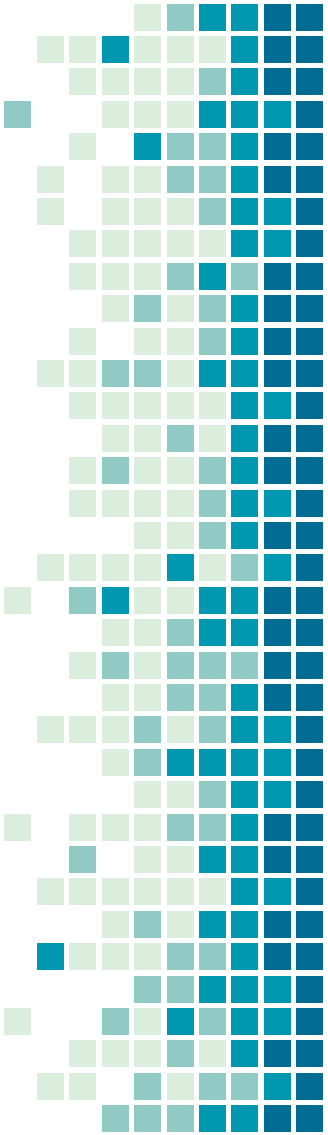
AMES prediction

Stability of the nitrenium ions, “nitrenium hypothesis”

pKa calculation

Finding Bioisosters of carbonic acids.

And more...



Basic Usage

single point calculation with RDKit

```
>>> from pygamess import Gamess
>>> from rdkit import Chem
>>> from rdkit.Chem import AllChem
>>> m = Chem.MolFromSmiles("CC")
>>> m = Chem.AddHs(m)
>>> AllChem.EmbedMolecule(m)
0
>>> AllChem.UFFOptimizeMolecule(m,maxIters=200)
0
>>> g = Gamess()
>>> nm = g.run(m)
>>> nm.GetProp("total_energy")
'-78.302511990200003'
```

optimize calculation with RDKit

Change run_type:

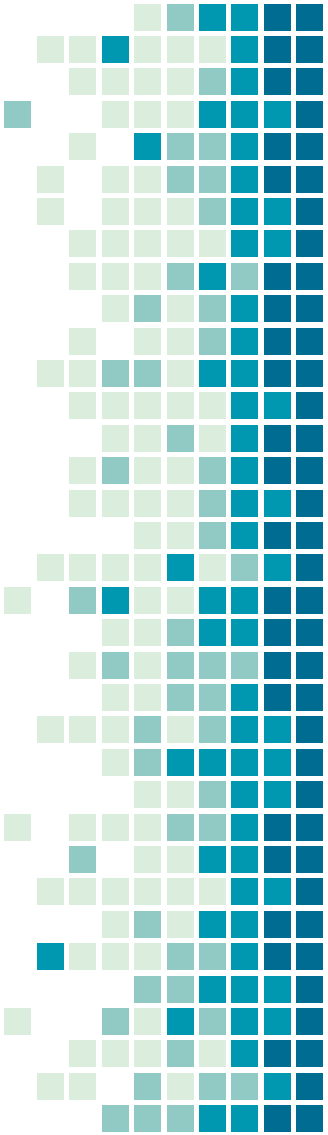
```
>>> from pygamess import Gamess
>>> from rdkit import Chem
>>> from rdkit.Chem import AllChem
>>> m = Chem.MolFromSmiles("CC")
>>> m = Chem.AddHs(m)
>>> AllChem.EmbedMolecule(m)
0
>>> AllChem.UFFOptimizeMolecule(m,maxIters=200)
0
>>> g = Gamess()
>>> g.run_type('optimize')
>>> optimized_mol = g.run(mol)
>>> optimized_mol.GetProp("total_energy")
'-78.306179626599999'
```

pygamess

Gamess wrapper for Python

Generating GAMESS input file from Chem object and execute quantum calculation.

Then returning Chem object generated from gamess output file.



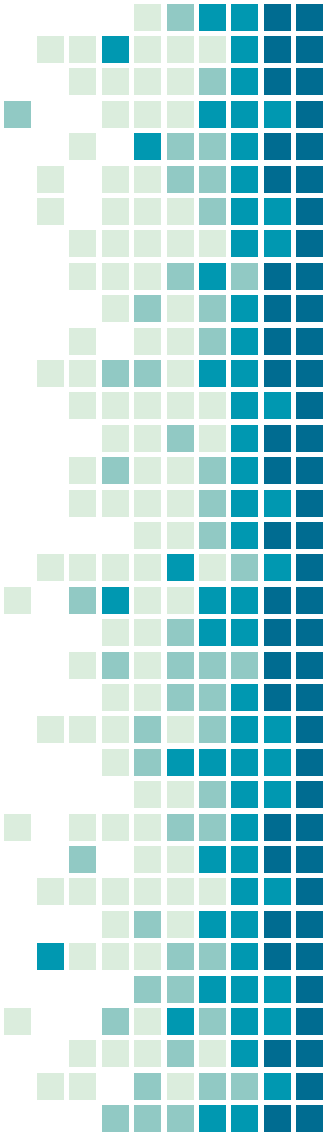
What is Gamess ?

The General Atomic and Molecular Electronic Structure System (GAMESS) is a general ab initio quantum chemistry package which is maintained by Gordon research group.

http://www.msg.ameslab.gov/gamess/

Why I choice gamess?

One reason is that it includes Fragment Molecular Orbital method (FMO) implementation, a powerfull method for SBDD.



History

0.4.1.1 (2017-09-16)

- Update Readme

0.4.1 (2017-09-16)

- Bug fixed (coordinates problem)

0.4.0 (2017-09-13)

- Change the backend lib 5 years... pybel to RDKit

0.3.0 (2012-03-31)

- Use internal rungms (default)
- Added basis_set method(STO-3G,3-21G,6-31G,6-311G,6-3
- Constructor can accept options
- Bug fixed (spin multiplicity)

0.2.2 (2012-03-30)

- Added charge settings
- Method name changed (gamess_input -> input)

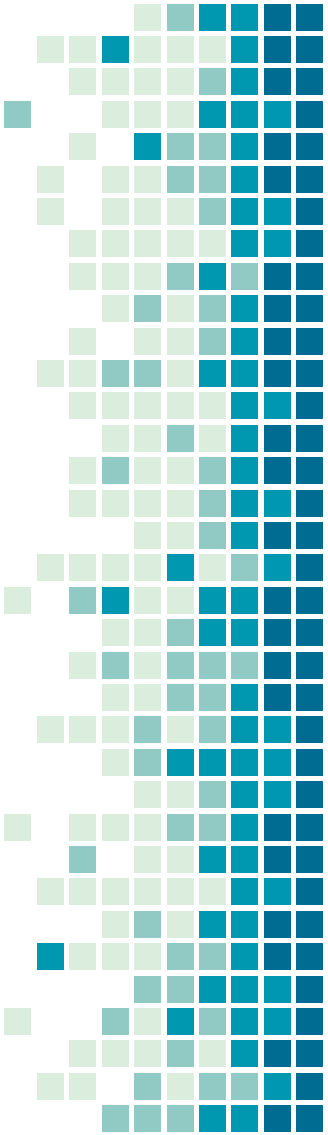
0.2.1 (2012-03-23)

- Bug fixed (multiplicity setting for pybel)
- Bug fixed (print error when rungms exec failed)

Now, I'm rewriting pygamess for integration with RDKit

Install:

pip install pygamess
(but GAMESS is required...)



Any suggestions and comments would be greatly appreciated. Thanks!

You can find me at:
Twitter: @fmkz___
Github: https://github.com/kzfm