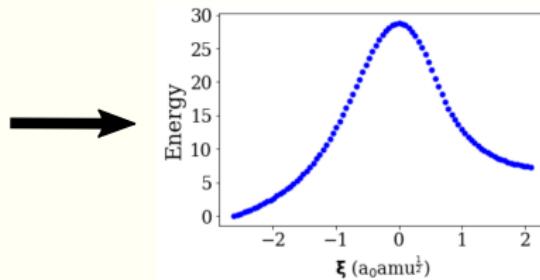


Exploring Chemical Reactions with Kudi

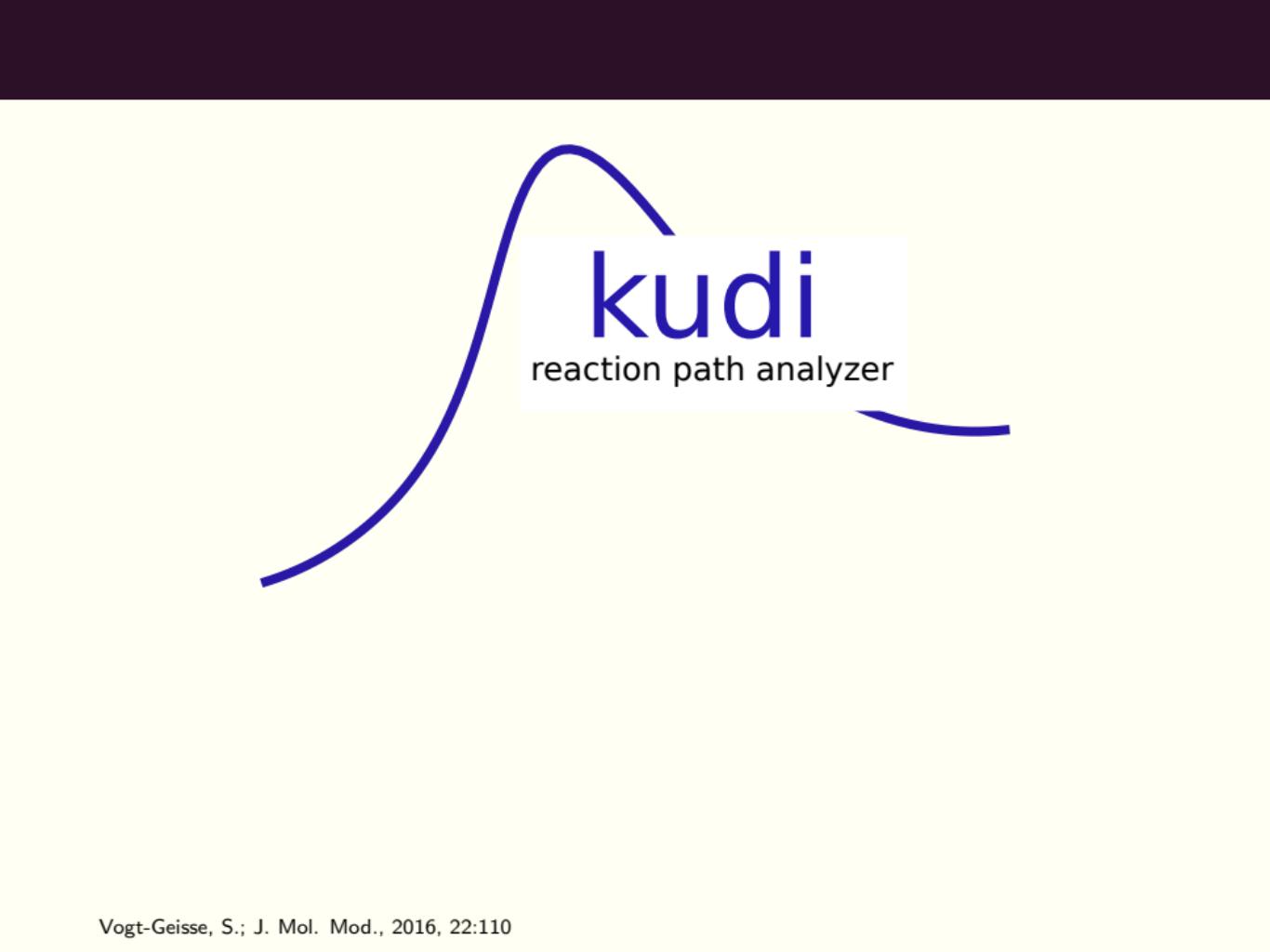
Stefan Vogt Geisse – Universidad de Concepción



Motivation



Kudi – Reaction Path Analyzer



kudi
reaction path analyzer

What does kudi mean?

kudi: grinding stone

Much like the native Mapuches used kudi to extract the maximum of nutrients from unprocessed grains, seeds and nuts, **kudi can be used as a tool to make the data contained in a chemical reaction path as available as possible.**



```
def parse_data(experiment):
    self.condition = None
    final_results = []
    for datum in experiment:
        final_result = self._process(datum)
        final_results.append(final_result)
    return final_results
```

Features

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- Currently works with Gaussian09, Orca4.0 and NBO6.0.
- Free for everyone! Available at
www.github.com/stvogt/kudi

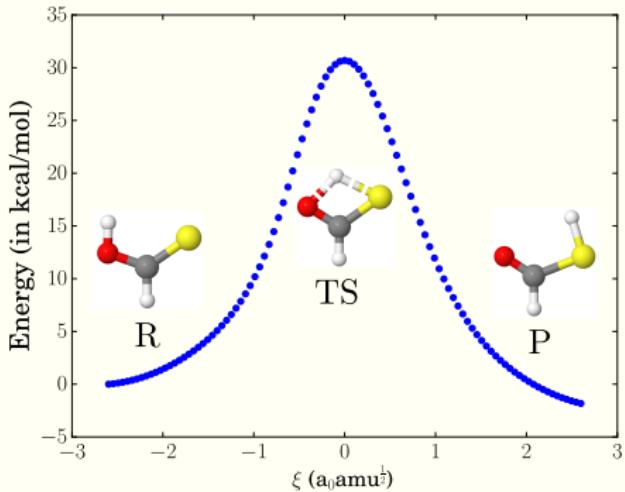
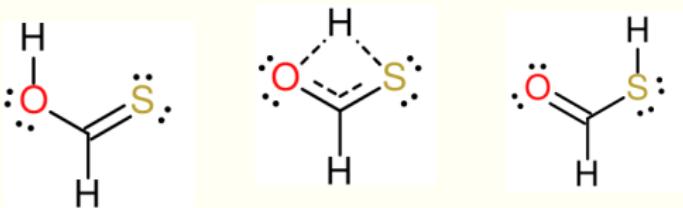
A minimal kudi script example

```
1  #! /usr/bin/python
2
3  import sys
4  from kudi import Path
5
6  outfile = sys.argv[1]
7  #outfile = "output.log"
8
9  ##Initiate Molecule object
10 Mol = Path(outfile)
11
12 # Saves XYZ coordinates in molden text or latex format
13 Mol.saveXYZ(format_="latex")
14
15 #Plot energy profile
16 energy = Mol.energy()
17 Mol.save("energy.dat",**energy)
18 Mol.savePlot('energy.svg', "Energy", **energy)
```

Obtaining bond distances and angles

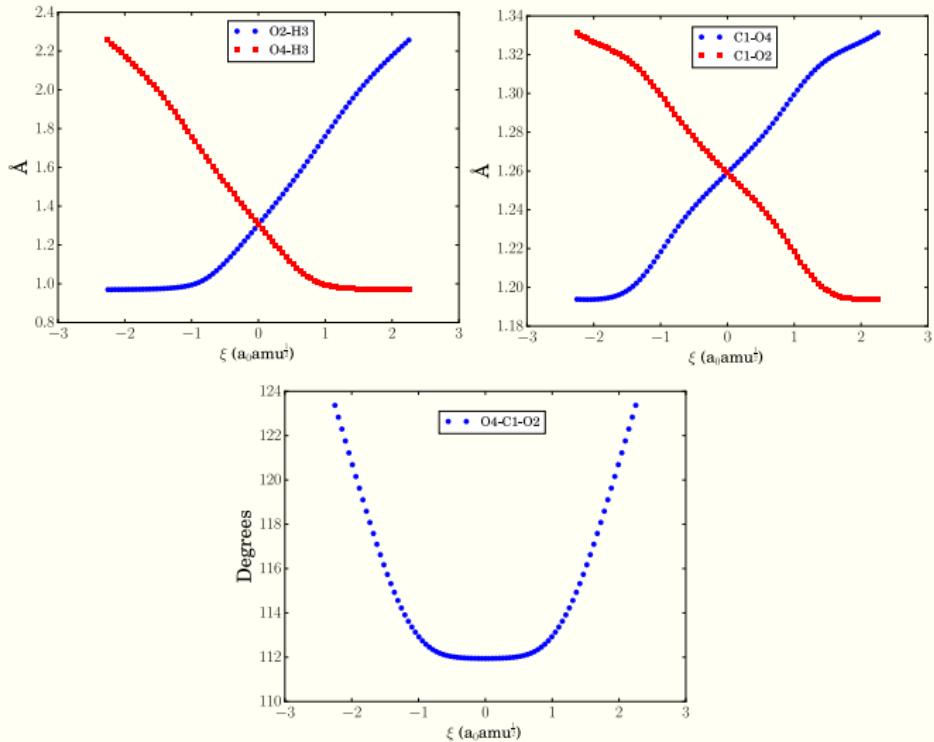
```
1  #! /usr/bin/python
2
3  import sys
4  from kudi import Path
5
6  outfile = sys.argv[1]
7
8  #Initiate molecule object
9  Mol = Path(outfile)
10
11 # Call distance object and specify distances
12 distances = Mol.distances(["C1-O2", "O2-H3", "O4-H3", "C1-O4"])
13 Mol.savePlotProps("sigma.svg", "\AA", ["C1-O2"], **distances)
14 Mol.savePlotProps("pi.svg", "\AA", ["O2-H3"], **distances)
15
16 # Call angle object and specify angles
17 angles = Mol.angles(["O4-C1-O2"])
18 Mol.savePlotProps("angles.svg", "Degrees", ["O4-C1-O2"], **angles)
```

Enol-Keto tautomerization in tioformic acid



Obtained using IRC at the PBE0/def2-TZVP level of theory

Structural changes



Electronic Chemical Potential (ECP)

The ECP can be calculated through finite differences and is related to Mulliken's definition of electronegativity:

$$\mu = -\frac{I + A}{2} = -\chi \quad (1)$$

μ measures the escaping tendency of the electronic cloud. Any difference of it drives electron transfer

Reaction electronic flux

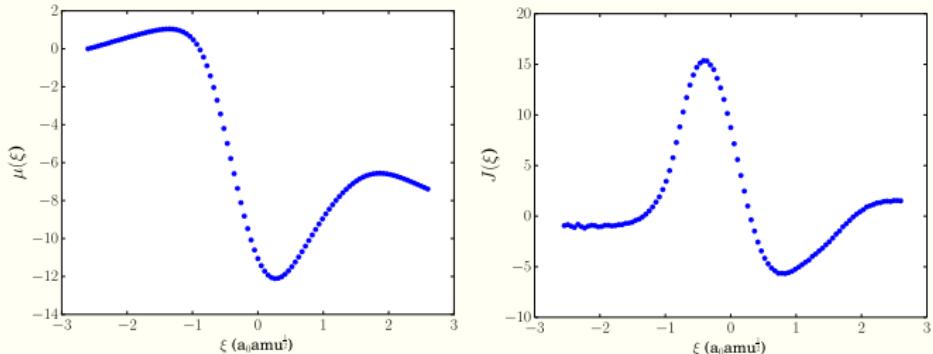
The reaction electronic flux is defined as the negative derivative of the chemical potential along a reaction coordinate:

$$J(\xi) = -\frac{d\mu(\xi)}{d\xi} \quad (2)$$

- $J(\xi) > 0 \longrightarrow$ delocalization
- $J(\xi) < 0 \longrightarrow$ localization

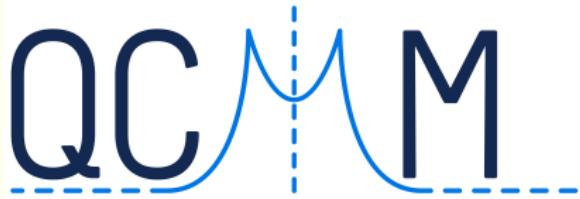
A good descriptor of electronic changes along a chemical reaction.

Electronic changes



Obtained using koopmans' approximation

Acknowledgments



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FONDECYT 1110949