

# Molecular Statistics, Week 1



**Jimmy Charnley Kromann**

Department of Chemistry

University of Copenhagen

2014

# Motivation



"I will never use this again"



# Motivation

Video



# Executing Python

python first\_program.py

Output

```
print "Hello World"

for i in range(5):
    print 'i', i
```

```
Hello World
1
2
3
4
```



# Programming in Python

- Variables and Datatypes
- Operators
- Comments
- Indentation
- Looping
- If-else
- Modules



# Variables and Datatypes

- String
- Integer
- Float
- List

```
name = "Peter"    # String
age = 31           # Integer
height = 1.80      # Float

#
s = [2, 4, 8, 16]
```



# Operators

Operator	Description
+	Addition
-	Subtraction
*	Multiplication
/	Division
%	Modulus
**	Exponent ( $a^b$ )

```
print 5.0 + 5.0
print 5.0 - 5.0
print 5.0 / 5.0
print 5.0 % 5.0
print 5.0**5.0

print 3 / 2
print 3.0 / 2.0
```



# Comments and Indentation





# Looping



# If and Else



# Modules



# First exercise



# The End

Exercise time

