CH40208: TOPICS IN COMPUTATIONAL CHEMISTRY

# INTRODUCTION TO PYTHON

### INTRODUCTION

- Aim is to give experience with computer programming in Python for computational chemistry applications
- Will build on the first and second year Python labs
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- Dr Andrew McCluskey
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#### **ASSESSMENT**

- x Dec: xx:xx Multiple Choice Questions and Error Spotting exercise
  - MCQs cover all of the material up to that date
  - Error spotting should be familiar from earlier work
  - Do not spend more than 30 minutes on either
- x Dec: xx:xx Programming test
  - Up to 3 hours
- ▶ Both parts are "open book" assessments; you may consult lecture notes, etc.

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## FIRST AND SECOND YEAR PYTHON

- Much of the first few weeks will feel like revision from first and second year
- More details and more opportunity for programming
  - Rather than filling in blanks
- If you would like to revise first or second year material, this should be available on moodle