

Lecture 1: Introduction to Python

Dr Benjamin J. Morgan¹ and Dr Andrew R. McCluskey^{1,2}

¹*Department of Chemistry, University of Bath, email: b.j.morgan@bath.ac.uk*

²*Diamond Light Source, email: andrew.mccluskey@diamond.ac.uk*

June 25, 2019

Aim

In this lecture, you will be introduced to Pythonic variable types, basic arithmetic, input and output (I/O) and intrinsic functions.

1 Introduction

The aim of this course is to develop skills in the use of computer programming (particularly in the Python programming language), building on the skills learned in the first and second year Computational Chemistry laboratory. You will then put these skills into practice, using Python to analyse chemical structures and perform quantum mechanical chemical calculations.

The Python programming language is one of the most popular programming languages in the world, ranking third on the TIOBE index¹ in June 2019,^C with the largest rate of change. Additionally,

References

- [C] T. T. S. Q. Company, *TIOBE Index for June 2019*, 2019, <https://www.tiobe.com/tiobe-index/>, [Online; accessed 2019-06-25].

¹The TIOBE index is an indicator of the popularity of a given programming language.