

Yonsei University Graduate Class

Energy Materials: Design, Discovery and Data Class Introduction & Overview

Prof. Aron Walsh

Department of Materials
Imperial College London



<https://wmd-group.github.io>



@lonepair

Class Outline

- 1. Introduction**
- 2. Course Overview**
- 3. How to use GitHub / Jupyter**

From London to Seoul

Aron Walsh

Professor at Imperial College London

Daniel Davies

PhD student at the University of Bath

Lucy Whalley

PhD student at Imperial College London

Aron Walsh – Background

Trinity College Dublin, Ireland

BA and PhD in Computational Chemistry

National Renewable Energy Laboratory, USA

Postdoc in Materials Physics (w/ Su-Huai Wei)

University College London, UK

Marie Curie Research Fellow (w/ Richard Catlow)

University of Bath, UK

Royal Society University Research Fellow

Imperial College London, UK

Professor in Materials Design

Aron Walsh – Background

Trinity College Dublin, Ireland

Structure-property relationships in metal oxides

National Renewable Energy Laboratory, USA

Photovoltaics and photoelectrochemistry

University College London, UK

Electroactive metal-organic frameworks

University of Bath, UK

Kesterite and perovskite solar cells

Imperial College London, UK

Theory of imperfect crystals

Republic of Ireland (1922)



1840: Population 8.3 million
1900: Population 4.5 million
2017: Population 6.5 million



Notable Scientists: Boyle / Hamilton / Walton / Boole / Kelvin / Stoney

Imperial College London (ICL)

(1851) Royal School of Mines

Government school for applied science

(1907) Imperial College

Founded as part of University of London

(2007) Imperial College London

Independent from University of London with
own medical and business schools

15000 Students (125 Countries)

Department of Materials

South Kensington

My office



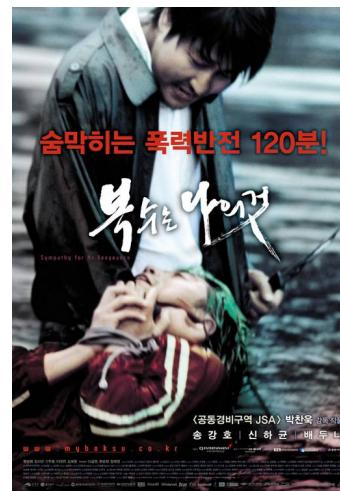
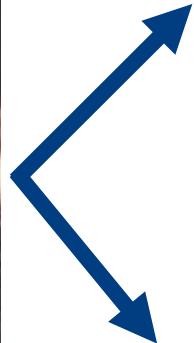
Class Question

Who has visited the UK?

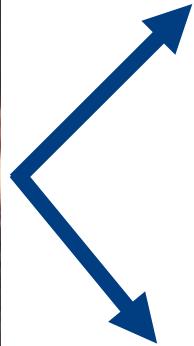
Trip #13 to South Korea



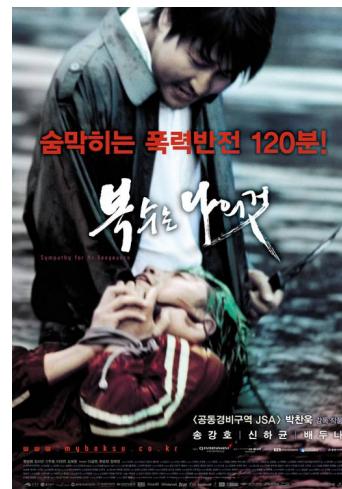
Trip #13 to South Korea



Trip #13 to South Korea



...



Class Introductions

- 1. Name**
- 2. Hometown**
- 3. Research Topic**

Class Outline

- 1. Introduction**
- 2. Course Overview**
- 3. How to use GitHub / Jupyter**

Course Concept – Repository

Energy Materials: Design, Discovery and Data

Overview

This intensive graduate course at Yonsei University aims to address challenges for developing materials for clean energy technologies. Using a combination of lectures and interactive practical sessions, we will cover:

Materials Design

- overview of semiconductor chemistry and physics
- materials science of solar energy conversion
- design principles for energy technologies

Materials Discovery

- first-principles materials modelling
- using Python for science and engineering
- identifying structures and compositions (via [Materials Project](#) and [SMACT](#))

Materials Data

- high-throughput screening
- processing and plotting data
- mining materials information

<https://github.com/wmd-group/yonsei2017>

Course Structure

(Mon – 3.4.17) Class Introduction & Overview

(Wed – 5.4.17) Semiconductor Chemistry & Physics

(Fri – 7.4.17) Solar Energy Conversion

(Mon – 10.4.17) Design Principles for Energy Technologies

(Wed – 12.4.17) Python for Science & Engineering

(Fri – 14.4.17) Exploring the Materials Hyperspace

(Mon – 17.4.17) Materials Theory & Simulation

(Wed – 19.4.17) Wrap-up, Quiz, and Party

Course Assessment

Attendance (25%)

Based on class register

Online Python Assignment (25%)

[Screenshot OR username to Youngkwang Jung]

Final Quiz (50%)

One question from each class

[Open book – access to notes]

Class Outline

- 1. Introduction**
- 2. Course Overview**
- 3. How to use GitHub / Jupyter**

Research #Protip

Useful Software

- 1. Slack** – group and project discussions
- 2. GitHub** – collaborate on codes and papers
- 3. Zenodo** – publish research data **#openscience**
- 4. Mendeley** – reference and share papers
- 5. Google Scholar** – your personal profile and tracking research papers (alerts)
- 6. Jupyter Notebook** – electronic lab book

Class Question

Does anyone have computer
programming experience?

e.g.

C / Fortran / Python / Matlab

Assignment: DataCamp

Free Lessons 1+2 (~ 1 hour)

<https://www.datacamp.com/courses/intro-to-python-for-data-science>

The screenshot shows the DataCamp website with a teal header. On the left, there's a logo with a person icon and the text "DataCamp We're hiring!". To the right are navigation links: Home, Courses, Tracks (beta), Pricing, Business, Community, Sign in, and a "Create Free Account" button. Below the header, the text "FREE COURSE" is displayed. The main title "Intro to Python for Data Science" is prominently shown in large white letters. A yellow button labeled "Start Course For Free" is below the title. To the right, there's a circular badge with "INTRODUCTION TO PYTHON" at the top and "PYTHON" at the bottom, featuring a green Python logo in the center. At the bottom of the page, there are statistics: 11 Videos, 57 Exercises, 4 hours, 146,373 Participants, and 4700 XP.

FREE COURSE

Intro to Python for Data Science

Start Course For Free

11 Videos 57 Exercises 4 hours 146,373 Participants 4700 XP

INTRODUCTION TO PYTHON

PYTHON

Let's Try GitHub

<https://github.com/WMD-group/yonsei17>