Using Assessment to Guide Student Learning

Kristi Closser

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Teaching Computation Online with MATLAB

FRESNO STATE®

Chemistry and Biochemistry

California State University, Fresno

- Part of the CSU system (23 campuses)
- 22,500 undergraduates, 2800 graduate/post-bac
- 88% from Central Valley
- 66% first generation
- Hispanic (HSI) and Asian-American Native American Pacific Islander (AANAPISI) serving institution

http://www.fresnostate.edu/academics/oie/data/index.html

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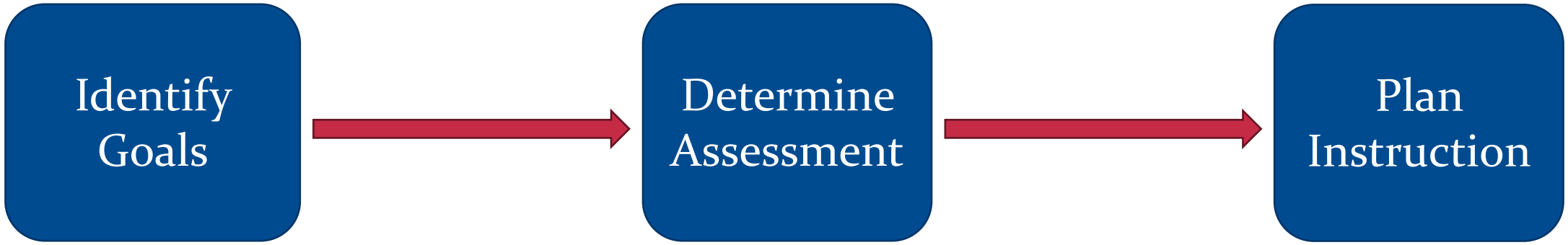
My Background

- Department of Chemistry and Biochemistry
- Research in theoretical chemistry
  - Excited electronic states of persistent organic pollutants
  - Quantum mechanics/density functional theory
- Teaching
  - General chemistry
  - Organic chemistry
  - Physical chemistry
  - Computational chemistry

Backwards Design



https://cft.vanderbilt.edu/guides-sub-pages/understanding-by-design/

Assessment Goals

- Summative
  - Collect information on student progress
  - Determine if learning outcomes have been met
- Formative
  - Provide feedback
  - Guide learning process

Effective assessment depends on clearly described learning objectives

https://cft.vanderbilt.edu/student-assessment-in-teaching-and-learning/

Physical Chemistry—Content based course

Upper division course, required for major

One course component: computational lab activities

- Students use mostly pre-generated code to analyze data and model concepts
  - Never require more than small code manipulations in live scripts (e.g. putting in a key equation, generating a plot)
  - Focus on concepts, code is just to support content
  - Build in issues where students are forced to think about what is happening with data (e.g. divide by 0 due to missing data)

Learning Obectives

Use active verbs: connect, create, solve

Be specific (example from teaching activity)

Learning Goals

Upon completion of this activity, students should accomplish the following

1. *Learning objectives within MATLAB*
    - Be familiar reading and running standard script files including basic code structure and comments
    - Explore statistical analysis functions available for data analysis such as min, max and std
    - Generate plots
2. *Learning objectives for Chemistry*
    - Analyze computational data from a database to extract information about titanium oxides
    - Assess the stability of materials and connect stability to stable structures.

https://serc.carleton.edu/teaching_computation/workshop_2020/activities/239528.html

Assessment

- Students submit answers to questions on handout
  - Evaluated for accuracy and completeness
    - Graded as satisfactory, progressing or incomplete
      - Satisfactory scores had all questions fully answered (roughly 70% correct)
      - Progressing scores allowed students to resubmit within a week
      - Incomplete scores mostly used if students did not submit at all.

- Informal discussions with students during class time were used to gauge understanding during the course of the activity

https://serc.carleton.edu/teaching_computation/workshop_2020/activities/239528.html

Teaching Activity

- Students worked through lab activity given a corresponding MATLAB script during class time
- MATLAB online used to ensure everyone had same version

Summary

Titanium dioxide (TiO_2) is an extremely common chemical substance and finds uses ranging from serving as a pigment for white paint, sunscreen and even toothpaste, to serving as a photosensitizer in waste water treatment processes where it initiates degradation of various organic molecule contaminants following exposure to UV light.

This activity explores the stability of various titanium oxide materials (TiO, TiO_2, Ti_2O_3, ...) using computed formation energies available from the open quantum materials database. This database contains structures and energies for a wide variety of materials that have been computed using density functional theory.

In completing this activity students are introduced to script files and data processing with MATLAB. The students run and modify a script which extracts data from an xml file containing formation energies of various titanium oxide compounds and then they must process and interpret the data using MATLAB.

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