## **Ab Initio Tools for Hypothesis Testing Workshop**

Proposers: Wendy Panero (Ohio State University) and Razvan Caracas (Ecole Normale Superior de Lyon)

Date: July 9, 2017 Location: Bear A

## Schedule

| Time          | Topics  | Speakers or Instructors   |
|---------------|---|---------------------------|
| 7:00am        | Breakfast   |                           |
| 7:30am        | Workshop check-in                                     |                           |
| 8:00-8:15am   | Welcome   | Panero                    |
| 8:15-9:30am   | Introduction to DFT                                   | Panero                    |
| 9:30-10:00am  | Coffee Break  | Tamaya Pre-function North |
| 10:00-12:00pm | Introduction to Calculation of Vibrational Properties | Caracas                   |
| 12:00–1:00pm  | Lunch   | Tamaya Pre-function North |
| 1:00-1:30pm   | The Raman RRUFF and WURM databases                    | Caracas                   |
| 1:30-5:00pm   | Hands on Workshop                                     | Panero and Caracas        |

- Check-in for the annual meeting begins at 4pm
- Welcome reception for the annual meeting begins at 4:30pm