

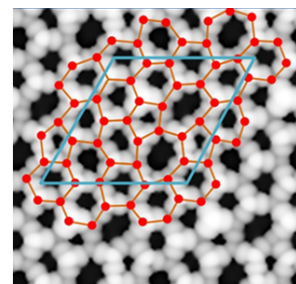


Workshop on
Theory and Computation for Interface Science and Catalysis:
 Fundamentals, Research and Hands on Engagement using VASP

Hosted at Brookhaven National Laboratory
 November 3-7, 2014

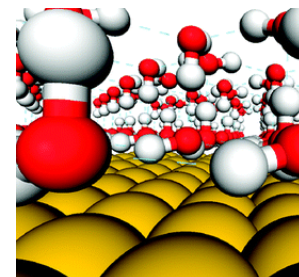
Workshop targeted for students and other researchers to

- Learn fundamentals and practical use of modern Density Functional Theory based computational tools
- Apply to research in interface science, catalysis and materials for energy applications
- Explore the cutting edge of evolutionary algorithms and data-driven approaches for materials discovery.

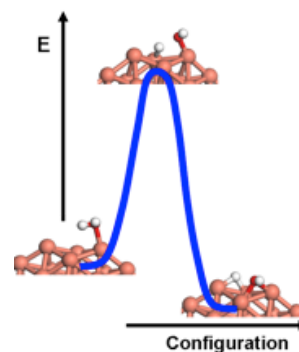


Morning lectures frame the subject, demonstrate experiments and theory working together in research, and introduce the theoretical methods. Speakers include:

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|--------------------------------------|-------------------------------|
| Cynthia Friend (Harvard) | Philip Allen (Stony Brook) |
| Jose Rodriguez (Brookhaven) | Ping Liu (Brookhaven) |
| Dion Vlachos (Delaware) | Mark Hybertsen (Brookhaven) |
| Jingguang Chen (Columbia/Brookhaven) | Annabella Selloni (Princeton) |
| Thomas Bligaard (SLAC/SUNCAT) | Artem Oganov (Stony Brook). |



Afternoon tutorials primarily will be hands-on experience with the VASP suite of tools led by Martijn Marsman (U. Vienna). Exercises will be executed on the computing cluster at the Center for Functional Nanomaterials, with tutorial support from the scientific staff in the Theory and Computation Group. Extensions to kinetic processes will be led by the Vlachos Group (Delaware). The interface to evolutionary algorithms will be led by the Oganov Group (Stony Brook).



Full program and registration details: <http://www.bnl.gov/theorycomp2014/>.

Workshop logistics:

- Program November 3 – 7, 2014
- Housing for all registrants on-site at Brookhaven at no cost
- Registration fee of \$300 covers all meals
- Registration deadline: Friday, October 3, 2014

Attendees are encouraged to consider future projects to enhance their research in particular computational studies that could be executed using CFN facilities under the User Program: <http://www.bnl.gov/cfn/user/>. CFN staff will be available for consultations and discussions of such future projects.

