

# NERSC Users Group 2013

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# What is NERSC?

- “The primary scientific computing facility for the Office of Science”
- Main facility is a Cray XE6 with ~150k cores
- Cray XC30 under construction
- IBM dataplex, ~10k cores
  - This is where they've stuck me
  - And I'm fine with that
- Also becoming a data repository

- Supercomputers are very different from batch clusters
  - It's all about the network
  - Scheduling is hard – 2-d packing problem
- Focused on MPI
  - Highly parallel
  - They expect you to run on  $\sim 1e4$  cores
  - For short times  $\sim 1hr$
- It's common for long jobs to checkpoint & restart

- Do I/O from a single node, distribute via MPI calls
- Monte-Carlo or event reconstruction could run well on this sort of setup
  - It would require some adjustment in thinking
  - And would probably underutilise the network

- They also have some more batch-like systems
  - But you have to pay for those
  - Staff is aware that some classes of users would like to see more of this
- They are will work with customers to customize solutions
- Planck got custom-managed hardware by pledging 2.5 FTEs to use it

- NEWT – RESTful API allowing access of NERSC resources through the web
  - Staff has used it to implement a lot of their own management tools
- Users are doing some really cool stuff with it
- Science gateways
  - QCD
  - Astronomy
  - Materials science
  - Climate

QUICK LINKS



Run No.

- [Runs](#)
- [Calibrations](#)
- [Plots](#)
- [DCS](#)
- [Tools](#)
- [System](#)

## Welcome to Daya Bay ODM

Enjoy monitoring ...

### Run List

- [All Completed Runs](#)
- [Ongoing Runs](#)
- [Last Week](#)
- [Last Month](#)
- [Monthly Archives](#)

### Run Type

- [Physics](#)
- [ADCalib](#)
- [WPCalib](#)
- [Pedastal](#)
- [FEEDiag](#)
- [MOMonitor](#)

### AD Calibration

- [<sup>68</sup>Ge](#)
- [<sup>60</sup>Co](#)
- [<sup>40</sup>K](#)
- [<sup>241</sup>Am<sup>13</sup>C + <sup>60</sup>Co](#)
- [<sup>241</sup>Am<sup>13</sup>C + <sup>68</sup>Ge](#)
- [ACU LED](#)
- [MO LED](#)
- [Double Pulse](#)
- [MCS](#)

### Run Tools

- [Search Run](#)
- [Statistics](#)
- [RSS: Latest Runs](#)

### DCS Monitor

- [DCS Chart](#)
- [EH1](#)
- [EH2](#)
- [EH3](#)

### Plots Search

- [Diagnostics](#)
- [PQM](#)
- [Simulation](#)



# MATERIALS PROJECT

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Accelerating materials discovery through advanced scientific computing and innovative design tools.

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## Database Statistics

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405 intercalation batteries 15175 conversion batteries

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### Materials Explorer

Search for materials information by chemistry, composition, or property.



### Lithium Battery Explorer

Find candidate materials for lithium batteries. Get voltage profiles and oxygen evolution data.



### Crystal Toolkit

Convert between CIF and VASP input files. Generate new crystals by substituting or removing species.



### Phase Diagram App

Computational phase diagrams for closed and open systems. Find stable phases and study reaction pathways.



### Reaction Calculator

Calculate the enthalpy of tens of thousands of reactions and compare with experimental values.



### Structure Predictor

Predict new compounds using data-mined substitution algorithms.

Find out more about our [open Materials API](#) and [pymatgen library](#) for querying large amounts of data.

## Tutorials



### Press Highlights

The New York Times

Beyond Fossil Fuels: Finding New Ways to Fill the Tank



The end of the petrolhead: Tomorrow's cars may just plug in



The Big Picture - Material Good



Building a better battery proves Material Genome Project's metal

all press

## Latest News

pymatgen v2.5.2

by Shyue Ping Ong - 22 hours ago

Version 2.5.2 of pymatgen has been released! Check out the change log at <https://pypi.python.org/pypi/pymatgen> for information on the latest changes.

pymatgen v2.5.2

The Materials Project is hiring!

A new year, a new pymatgen

Journal article on the Python Materials Genomics library

all entries

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- LSST DESC was granted 2.5M hours
- Initial use is raytracing the telescope
  - Lots of variation in job runtimes makes it hard to schedule
- Hoping to use NEWT to run pipeline jobs at NERSC, controlled from SLAC
- Will need to set up parallel jobs that act as virtual batch farms
  - e.g. Reserve 32 nodes for 24 hours
  - Use a (somewhat experimental) queueing system taskfarmerMQ