

# Turn-key solutions with AiiDA lab

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# The rise of simulation science

## 2013 Chemistry Prize



**Taking the  
Experiment to  
Cyberspace**

The Nobel Prize in Chemistry 2013



Photo © Harvard University

### **Martin Karplus**

Martin Karplus, U.S. and Austrian citizen. Born 1930 in Vienna, Austria. Ph.D. 1953 from California Institute



Photo: S. Fisch

### **Michael Levitt**

Michael Levitt, U.S., British and Israeli citizen. Born 1947 in Pretoria, South Africa. Ph.D. 1971 from



Photo: Wikimedia Commons

### **Arie Warshel**

Arie Warshel, U.S. and Israeli citizen. Born 1940 in Kibbutz Sde-Nahum, Israel. Ph.D. 1969 from

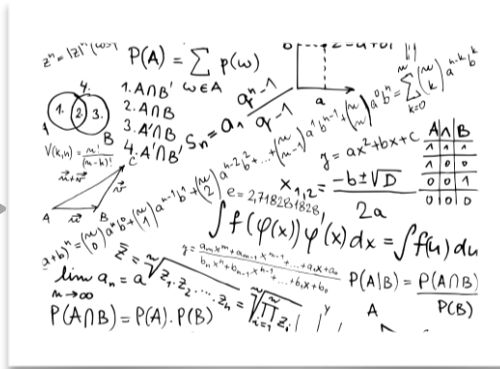
“The prize focuses on how to evaluate the variation in the energy of the real system in an accurate and efficient way.”

“Simulations are so realistic that they predict the outcome of traditional experiments.”

# Three pillars of science

- > Pillar I : experiment. Mostly done by experimentalists.
- > Pillar II : theory. Mostly done by theoretical and computational scientists.
- > Pillar III: simulation. Mostly done by computational scientists.

*can be seen as a merging point between theory and experiment*



# Motivation: knowledge transfer

**Science is evolving as a collaboration between theory and experiment, however the means of communication between the two parts are rather inefficient:**

- > Experimentalists are the ones who can verify theoretical models against the measured data. Are they aware of the simulation tools that computational scientists are developing?
- > How would do we setup communications between computational scientists and experimentalists?
  - > PDF report via email?
  - > Presentation?
- > How much time would you spend converting your data in different data formats, different units and prepare them to look as they should be?
- > Would you like to/be able to instruct your experimental collaborator to run calculations (Quantum ESPRESSO, CP2K, ..) ?

# AiiDA vs AiiDA lab

Computational scientist

Computational/Experimental  
scientist





- > Can run complex workflows
- > Stores selected data
- > Stores data provenance
- > Has Python or command line interface





- > Fully integrated with AiiDA
- > User-friendly web interface (Jupyter notebooks & widgets)
- > Easy application development (directly in Python)
- > Collaborative environment.
- > Handy visualisation and editing tools
- > App Store for sharing applications


# AiiDA lab Home Page

  
File Manager

  
Terminal

  
Tasks

  
App Store

  
Help

✔ Latest Version

Manage App

URL

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**▼ Empa nanotech@surfaces Laboratory - Graphene nanoribbons**

**Structures**

- Upload structures
- Scale structures
- Construct cell
- Assign spin, remove atoms

**Nanoribbons**

- Submit calculation
- Search database

✔ Latest Version

Manage App

URL

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**▼ LSMO apps**

**Isotherm**

- Compute one
- Compute Henry Coefficient
- Analyse the results

**Pore analysis**

- Pore Analysis

**Geometry Optimization**

- Geometry Optimization
- Geometry Optimization and Charges

**Computers/Codes**

- Setup

✔ Latest Version

Manage App

URL

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**▼ AiIDA lab Widgets**

**Basic data objects.**

- Dealing with one structure
- AiIDA datatypes viewers

**Codes and computers.**

- Setup computer
- Setup code
- Dealing with codes and computers

✔ Latest Version


Manage App

URL

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**▼ Quantum ESPRESSO**

⚠ Update Available


QUANTUMESPRESSO

Manage App

URL

# App Manager

/ home / appstore / aiidalab-lsmo

LSMO

LSMO apps

Authors: A. Yakutovich

Description: Applications from the LSMO group

URL: <https://github.com/lsmo-epfl/aiidalab-epfl-lsmo.git>

Release line

che\_609\_course

Installed version

2cbf398e14c9e643dc02f462ff

Uninstall

Install

Update

☒ There are local modifications.

☐ Ignore

**Tight connection with Git for installation/deinstallation, update, version selection.**



# Running calculations and analysing results

The screenshot displays the AiiDAlab web interface in a browser window. The address bar shows the URL: <https://aiidalab.materialscloud.org/user/aliaksandr.yakutovich@epfl.ch/apps/apps/home/start.ipynb>. The interface features a top navigation bar with the AiiDAlab logo and buttons for 'Edit App', 'Logout', 'Control Panel', and 'Materials Cloud'. Below this, a row of icons provides access to 'File Manager', 'Terminal', 'Tasks', 'App Store', and 'Help'. The 'App Store' section is currently active, displaying a grid of application categories. Each category includes a list of tasks and a 'Manage App' button. The 'LSMO apps' section includes 'Isotherm', 'Pore analysis', and 'Geometry Optimization'. The 'AiiDA lab Widgets' section includes 'Basic data objects.', 'Codes and computers.', and 'Processes.'. The 'Quantum ESPRESSO' section is partially visible at the bottom. A green checkmark and the text 'Latest Version' are displayed next to the 'Geometry Optimization' category.

File Manager Terminal Tasks App Store Help

Manage App URL

▼ LSMO apps

✓ Latest Version

**Isotherm**

- Compute one
- Compute Henry Coefficient
- Analyse the results

**Pore analysis**

- Pore Analysis

**Geometry Optimization**

- Geometry Optimization
- Geometry Optimization and Charges

Manage App URL

▼ AiiDA lab Widgets

✓ Latest Version

**Basic data objects.**

- Dealing with one structure
- AiiDA datatypes viewers

**Codes and computers.**

- Setup computer
- Setup code
- Dealing with codes and computers

**Processes.**

- Process list
- Follow a process

Manage App URL

▼ Quantum ESPRESSO



Before AiiDA lab the typical questions from experimental scientists would be:

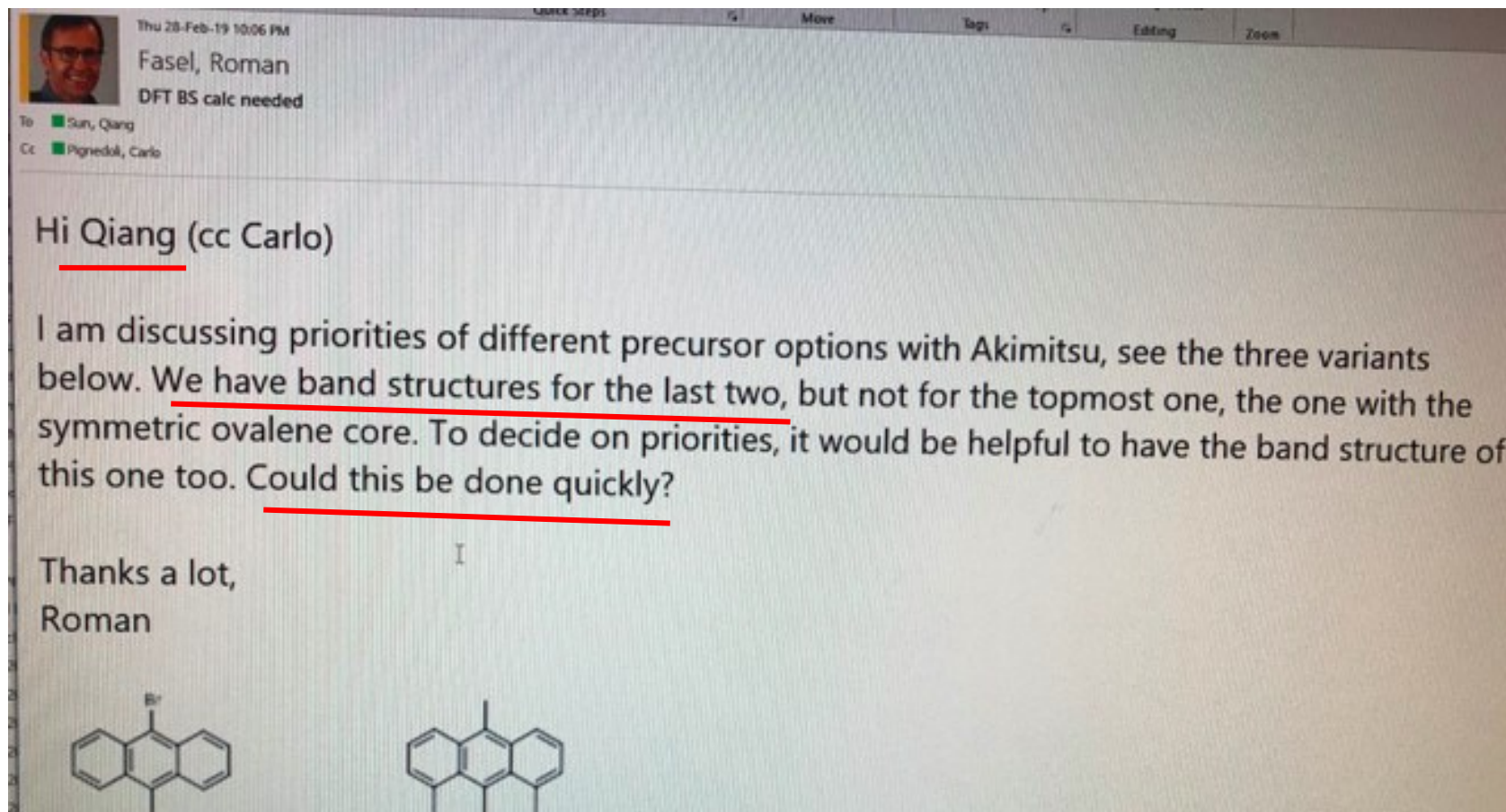
- > Some while ago\* we discussed ribbons A, B, C. Did you compute the band structure?
- > Does it take long to have the band structure of ...?

\* can be more than 1 year ago.



# Example from Empa

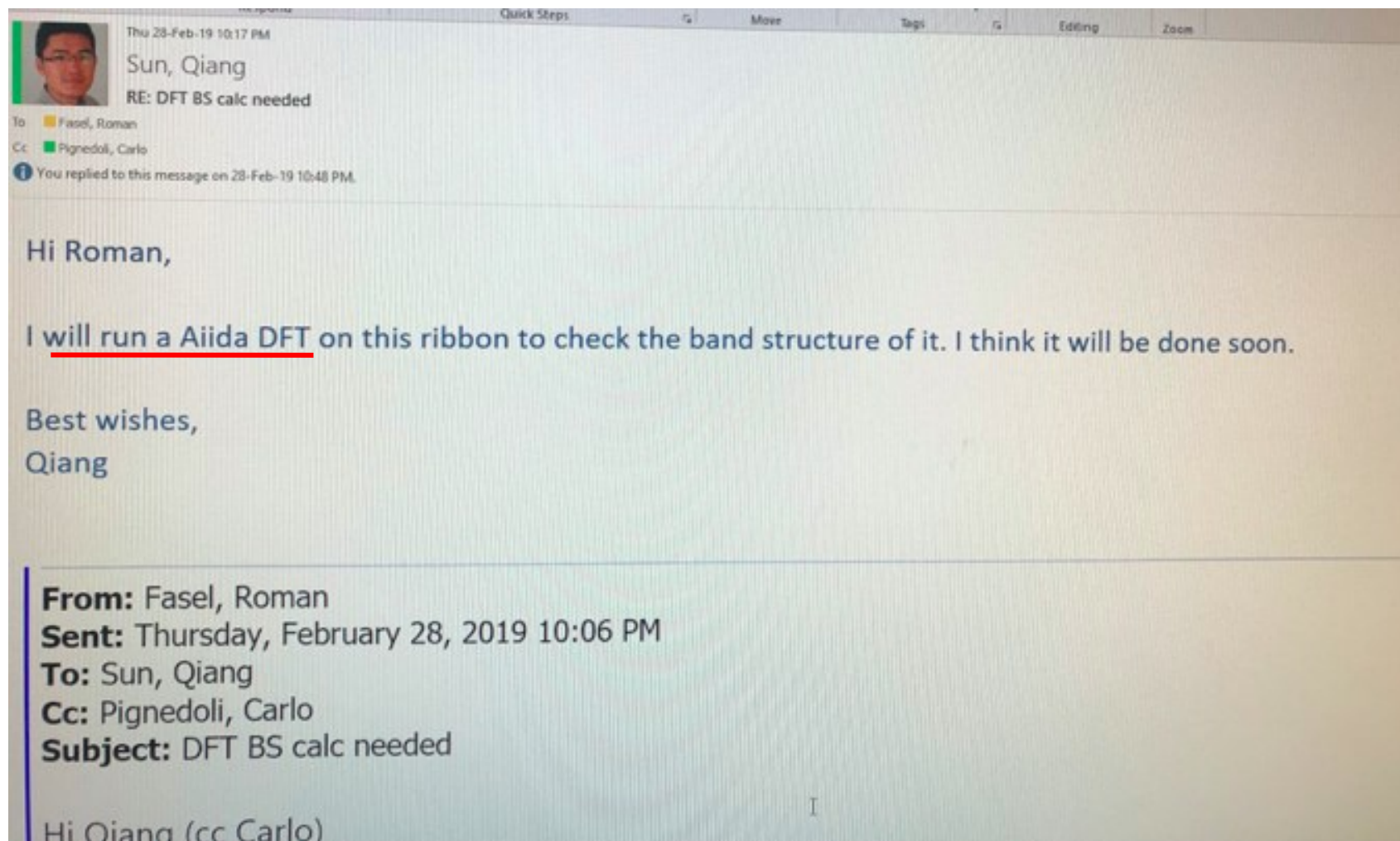
... now



- > Request to run calculations directly addressed to an Exp Phd
- > Status of available calculations known
- > Implicitly expecting this will be fast

# Example from Empa

... now



> No support needed.

# Browsing electronic structure results

The screenshot displays the AiiDAlab web interface in a browser window. The address bar shows the URL: `https://dev-aiidlab.materialscloud.org/user/carlo.pignedoli@empa.ch/apps/apps/home/start.ipynb?`. The interface features a top navigation bar with the AiiDAlab logo and links for 'Edit App', 'Logout', 'Control Panel', and 'Materials Cloud'. Below this, a row of icons represents 'File Manager', 'Terminal', 'Tasks', 'App Store', and 'Help'. A notification 'Update Available' is present in the top right. The main content area is divided into two sections, both for the user 'Empa nanotech@surfaces Laboratory'. The first section, 'Scanning Probe Microscopy', includes a 'General' tab with 'Setup codes' and 'Manage calculations', and sub-tabs for 'STM', 'ORB', 'PDOS', and 'AFM', each with 'Submit' and 'View' options. The second section, 'On-Surface Chemistry', includes a 'Calculations' tab with 'Submit optimizations and GW', 'Build slab', 'Search opt. slabs', 'Search opt. molecules', and 'Search opt. bulks', and sub-tabs for 'Constr. opt. chains' and 'Nudged elastic band', each with 'Generate replicas', 'Search replica chains', 'Submit NEB', and 'Search NEBs' options. Both sections have 'Manage App' and 'URL' buttons and a 'Latest Version' indicator. Vertical double-headed arrows are visible on the right side of each section.

start-154

https://dev-aiidlab.materialscloud.org/user/carlo.pignedoli@empa.ch/apps/apps/home/start.ipynb?

AiiDAlab

Edit App Logout Control Panel Materials Cloud

Update Available

File Manager Terminal Tasks App Store Help

Manage App URL

Empa nanotech@surfaces Laboratory - Scanning Probe Microscopy

Latest Version

General

- Setup codes
- Manage calculations

STM

- Submit STM
- View STM

ORB

- Submit ORB
- View ORB

PDOS

- Submit PDOS
- View PDOS

AFM

- Submit AFM
- View AFM

HR-STM

- Submit HR-STM
- View HR-STM

Manage App URL

Empa nanotech@surfaces Laboratory - On-Surface Chemistry

Latest Version

Calculations

- Submit optimizations and GW
- Build slab
- Search opt. slabs
- Search opt. molecules
- Search opt. bulks

Constr. opt. chains

- Generate replicas
- Search replica chains

Nudged elastic band

- Submit NEB
- Search NEBs

ASCALE  
TION

- > **(collaboration)** AiiDA lab provides an environment where people with different expertise can collaborate on a common computational project.
- > **(saving time, avoiding mistakes)** Using AiiDA lab one can directly exchange the simulation results in an appropriate format boosting know-how transfer.
- > **(modularity)** Modularity of AiiDA lab allows to easily build powerful tools by combining compact well-defined components.



DRIVING THE EXASCALE TRANSITION

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THANKS