

Turn-key solutions with AiiDA lab

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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

Arieh Warshel

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

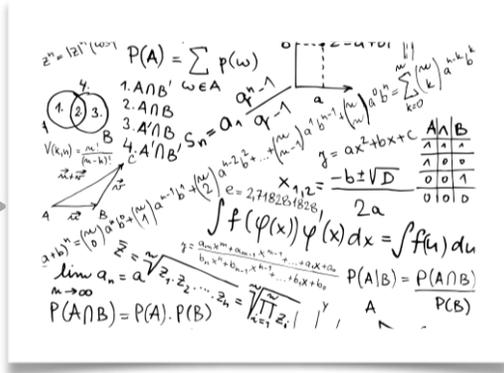
“The prize focuses on how to evaluate the variation in the energy of the real system in an accurate and efficient way.”

“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

The screenshot shows the AiiDA lab Home Page with a navigation bar at the top containing icons for File Manager, Terminal, Tasks, App Store, and Help. Below the navigation bar are four main application categories, each with a list of sub-features and a 'Manage App' button:

- Empa nanotech@surfaces Laboratory - Graphene nanoribbons** (Latest Version): Structures (Upload structures, Scale structures, Construct cell, Assign spin, remove atoms), Nanoribbons (Submit calculation, Search database).
- 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), Computers/Codes (Setup). The 'Manage App' button is circled in red.
- 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).
- Quantum ESPRESSO** (Update Available): Includes the Quantum ESPRESSO logo.

App Manager

The screenshot shows the App Manager interface for the LSMO app. The breadcrumb path is `/home / appstore / aiiDALab-lsmo`. The app details are:

- 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` (selected in a dropdown menu)
- Installed version:** `2cbf398e14c9e643dc02f462ff`
- Actions:** Uninstall (red button), Install (grey button), Update (green button)
- Options:** There are local modifications. Ignore

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



Running calculations and analysing results

The screenshot shows the AiiDAlab web interface in a browser window. The URL is <https://aiidalab.materialscloud.org/user/aliaksandr.yakutovich@epfl.ch/apps/apps/home/start.ipynb>. The interface includes a navigation bar with 'Edit App', 'Logout', 'Control Panel', and 'Materials Cloud' buttons. Below the navigation bar are icons for 'File Manager', 'Terminal', 'Tasks', 'App Store', and 'Help'. The 'Help' icon has a 'Manage App' button and a 'URL' button next to it. The main content area is divided into two sections: 'LSMO apps' and 'AiiDA lab Widgets'. The 'LSMO apps' section is expanded and shows three categories: 'Isotherm', 'Pore analysis', and 'Geometry Optimization'. Each category has a list of tasks and a 'Manage App' button. The 'AiiDA lab Widgets' section is also expanded and shows three categories: 'Basic data objects.', 'Codes and computers.', and 'Processes.'. Each category has a list of tasks and a 'Manage App' button. The interface also features a 'Latest Version' indicator for each section.

Navigation Bar: Edit App, Logout, Control Panel, Materials Cloud

Main Navigation: 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

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

Quantum ESPRESSO

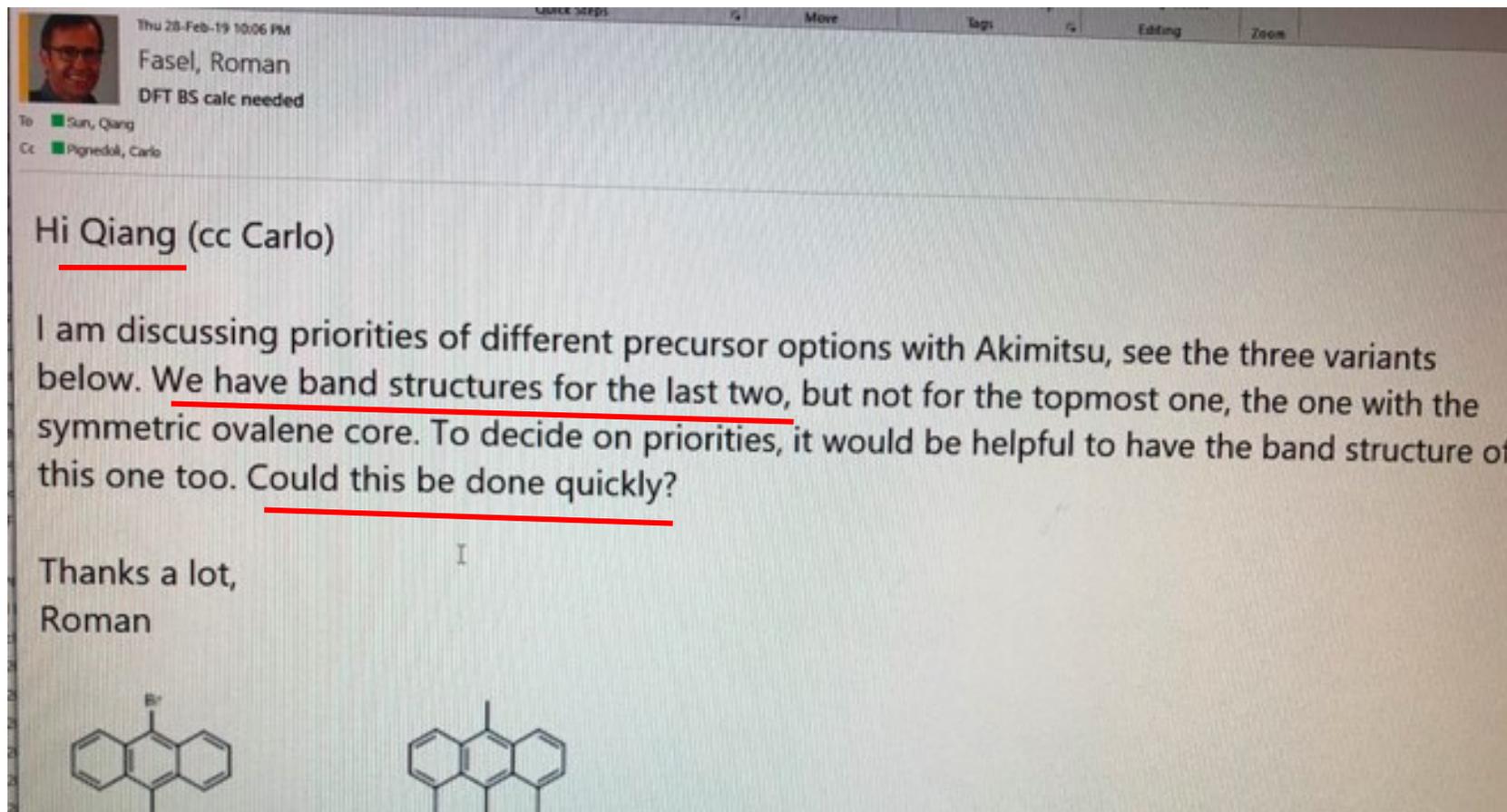
Before AiiDA lab the typical questions from experimental scientists would be:

- > 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

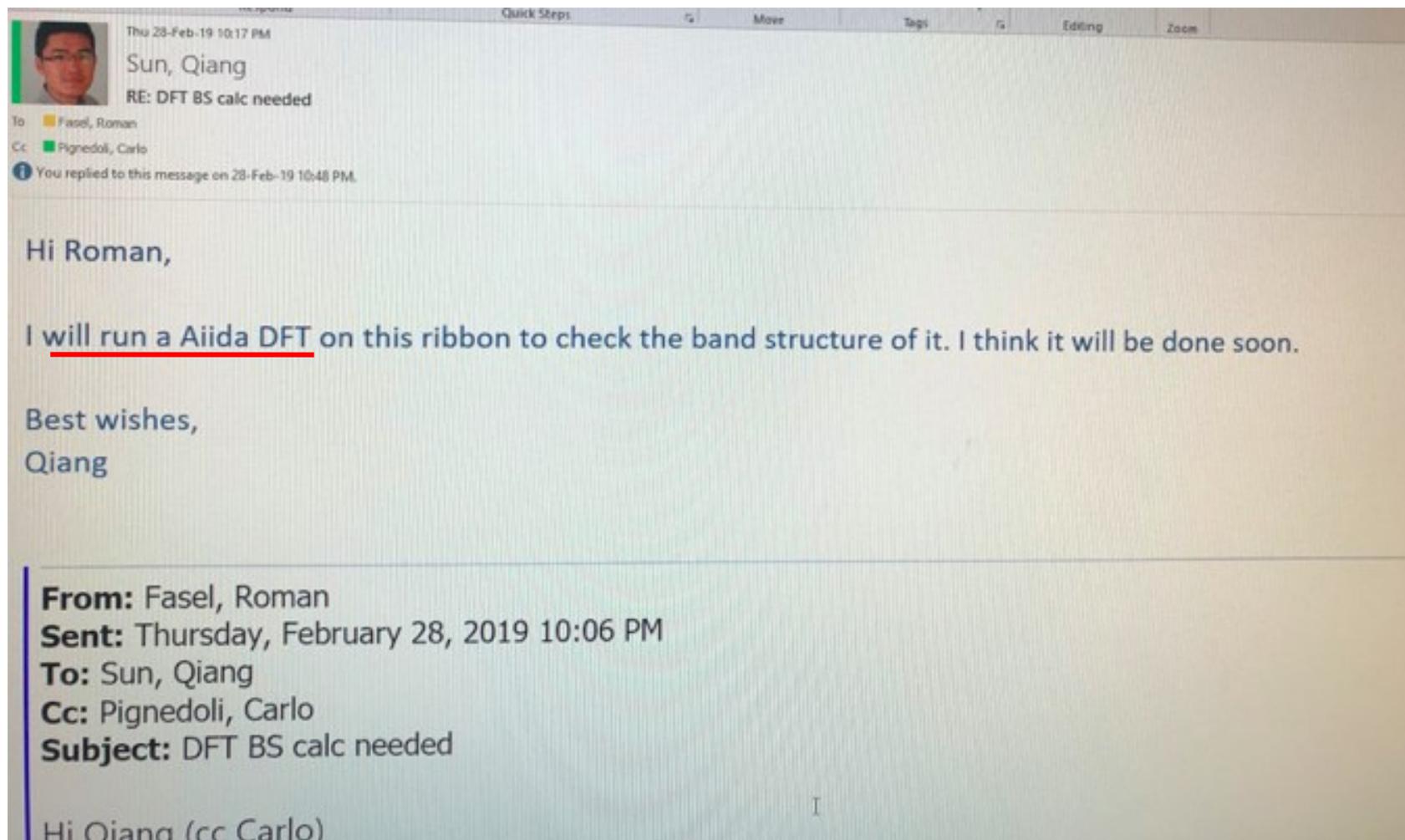
... now



- > 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 shows the AiiDAlab web interface. At the top, there is a navigation bar with the AiiDAlab logo and links for 'Edit App', 'Logout', 'Control Panel', and 'Materials Cloud'. Below this is a row of icons for 'File Manager', 'Terminal', 'Tasks', 'App Store', and 'Help'. A notification 'Update Available' is visible in the top right. The main content area is divided into two sections, each representing a different application.

Empa nanotech@surfaces Laboratory - Scanning Probe Microscopy

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

Buttons: Manage App, URL

Empa nanotech@surfaces Laboratory - On-Surface Chemistry

Calculations

- Submit optimizatons 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

Buttons: Manage App, URL

- > **(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