Turn-key solutions with AiiDA lab

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DRIVING
THE EXASCALE
TRANSITION

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."

MAX DRIVING THE EXASCALE TRANSITION

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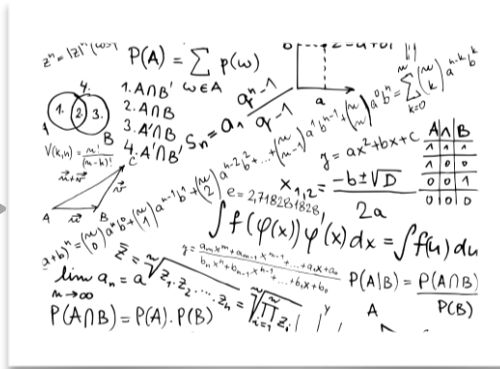
Science is evolving as a collaboration between theory and experiment, however the means of communication between the two parts are rather inefficient:

> 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

AiiDA

> Can run complex workflows

> Stores selected data

> Stores data provenance

> Has Python or command line interface

AiiDAlab

> 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

AiiDA lab Home Page

App Manager

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

 for sharing

Running calculations and analysing results

Before AiiDA lab the typical questions from experimental scientists would be:
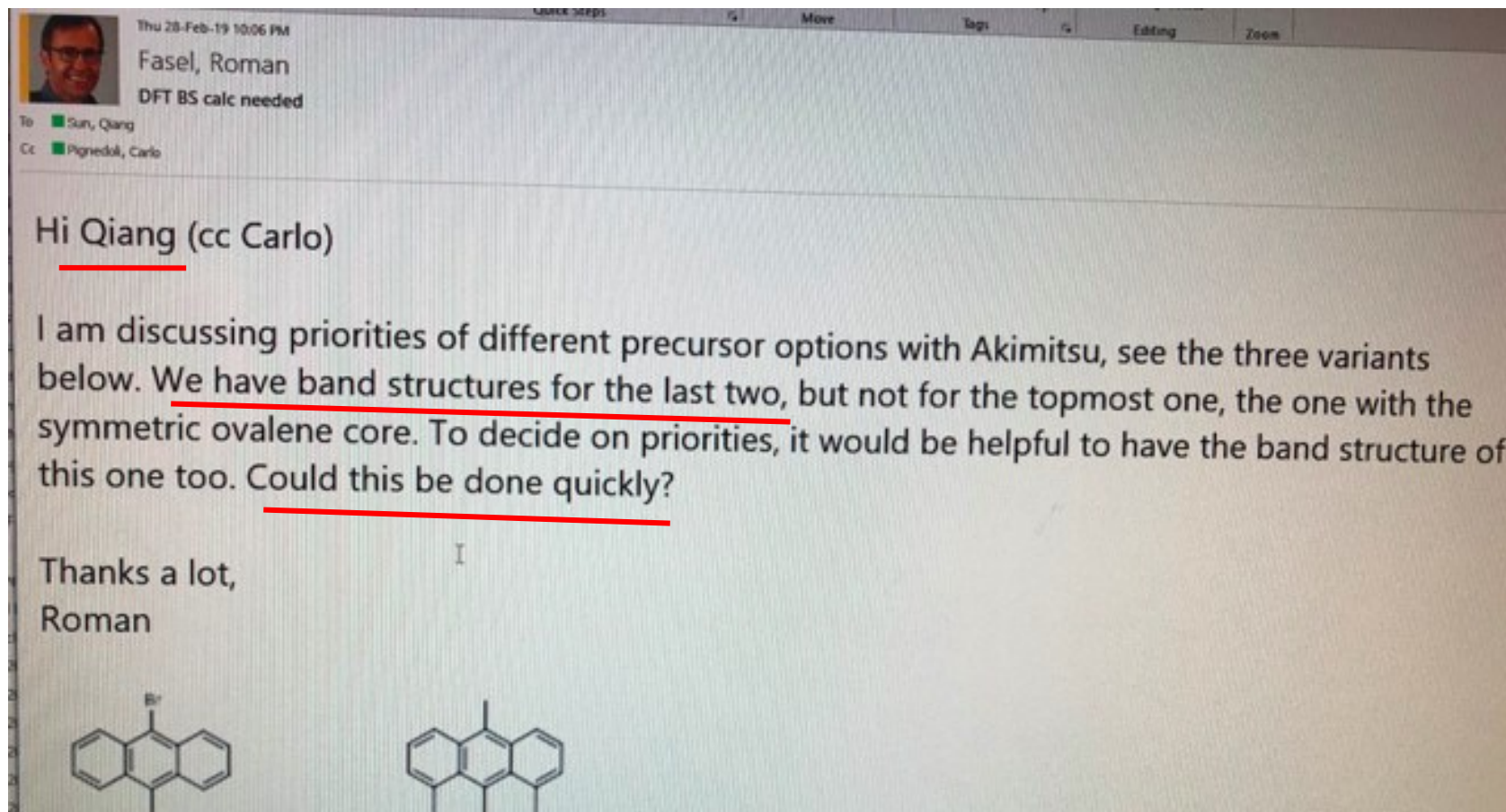
> Some while ago* we discussed ribbons A, B, C. Did you compute the band structure?

> Does it take long to have the band structure of …?
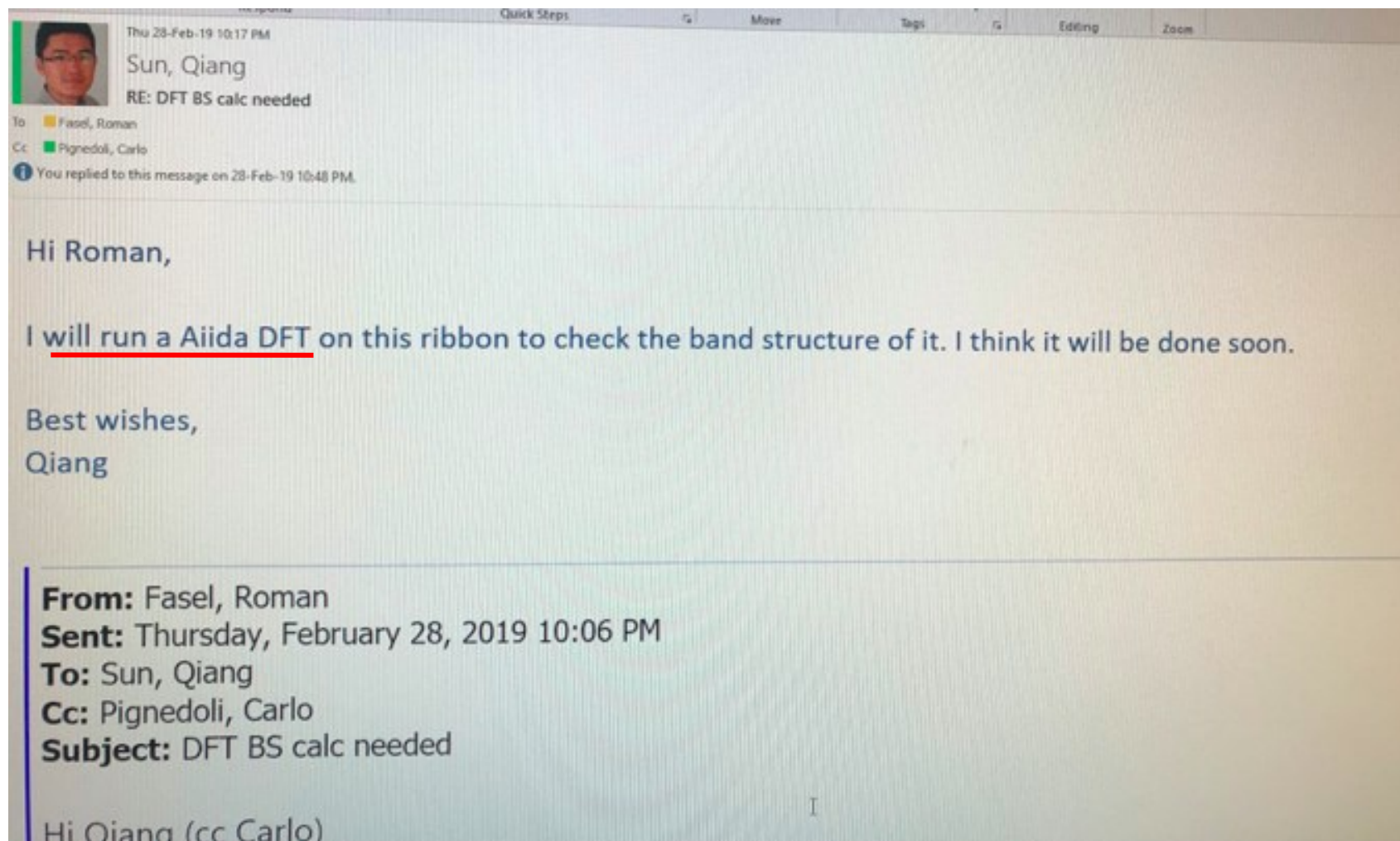
* can be more than 1 year ago.

Example from Empa

... now

Thu 28-Feb-19 10:06 PM

Fasel, Roman

DFT BS calc needed

To Sun, Qiang
Cc Pignedoli, Carlo

Hi Qiang (cc Carlo)

I am discussing priorities of different precursor options with Akimitsu, see the three variants below. We have band structures for the last two, but not for the topmost one, the one with the symmetric ovalene core. To decide on priorities, it would be helpful to have the band structure of this one too. Could this be done quickly?

Thanks a lot,
Roman

> 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

> **(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.

THANKS

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