VISTA Seminar

Seminar 42

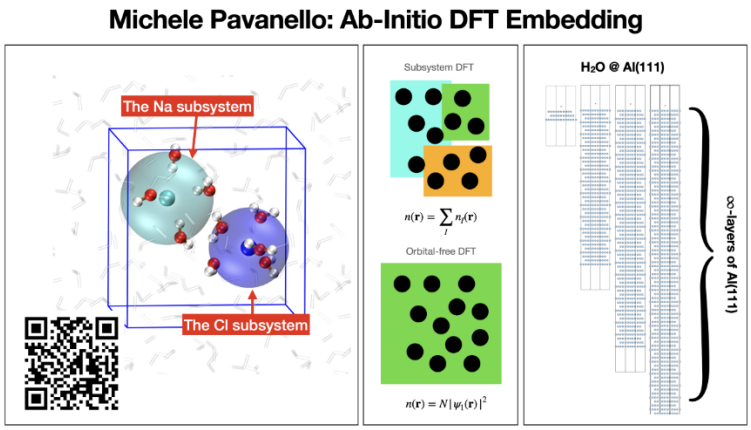
October 5, 2022

10:00 am – 11:30 am EDT / 3:00 – 4:30 BST / 4:00 pm – 5:30 pm Paris

TOC:

Cracking Challenging Electronic Structures: Embedding, machine learning and orbital-free DFT are the key

Michele Pavanello
Rutgers University-Newark, USA
Email: m.pavanello@rutgers.edu



Challenging electronic structures are of two types: (1) Large systems, too large for conventional electronic structure methods, (2) Strongly correlated electrons, where a mean-field treatment of the electronic systems is inadequate. In this talk I will show that a combination of embedding, orbital-free DFT, Kohn-Sham (KS)-DFT and machine learning successfully tackles both challenges for such systems as molecular condensed phases and interfaces of sizes untouchable by mainstream methods. My talk will focus on nonstandard embedding workflows of recent formulation. These include embedding KS-DFT subsystems in orbital-free DFT for the improved treatment of interfaces involving metallic systems. We also developed a machine learning (ML) method where the learned quantity is the one-electron reduced density matrix. Exploiting the theorems of reduced density matrix functional theory, we learn KS-DFT as well as post-Hartree-Fock methods delivering accurate predicted electronic structures, energies and forces for ab-initio molecular dynamics simulations in record wall-times. To make the methods available to the broader community, in the past 3 years we produced Python implementations of electronic structure solvers in plane wave basis based on Quantum ESPRESSO (QEpy) as well as ML-based solvers (QMLearn), orbital-free DFT (DFTpy) and density embedding (eDFTpy). With this arsenal at our disposal, we are ready to tackle the most difficult and timely electronic structure challenges.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 42
Time: Oct 5, 2022 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting
https://buffalo.zoom.us/j/91897705724?pwd=NXlCSXd3RlZFU1lDY0RNRTZiUUp0QT09

Meeting ID: 918 9770 5724
Passcode: 921543
One tap mobile
+16465588656,,91897705724#,,,,*921543# US (New York)
+13017158592,,91897705724#,,,,*921543# US (Washington DC)

Dial by your location
- +1 646 558 8656 US (New York)
- +1 301 715 8592 US (Washington DC)
- +1 312 626 6799 US (Chicago)
- +1 346 248 7799 US (Houston)
- +1 669 900 9128 US (San Jose)
- +1 253 215 8782 US (Tacoma)

Meeting ID: 918 9770 5724
Passcode: 921543
Find your local number: https://buffalo.zoom.us/u/an0oEUPte

Join by SIP
91897705724@zoomcrc.com

Join by H.323
162.255.37.11 (US West)
162.255.36.11 (US East)
115.114.131.7 (India Mumbai)
115.114.115.7 (India Hyderabad)
213.19.144.110 (Amsterdam Netherlands)
213.244.140.110 (Germany)
103.122.166.55 (Australia Sydney)
103.122.167.55 (Australia Melbourne)
149.137.40.110 (Singapore)
64.211.144.160 (Brazil)
69.174.57.160 (Canada Toronto)
65.39.152.160 (Canada Vancouver)
207.226.132.110 (Japan Tokyo)
149.137.24.110 (Japan Osaka)
Meeting ID: 918 9770 5724
Passcode: 921543