

Machine Learning in Electronic Structure and Molecular Dynamics



16 - 20 May 2022
Kigali - Rwanda

Further information:
<http://indico.ictp.it/event/9787/>
smr3702@ictp.it

This is the culminating workshop of the Machine Learning (ML) in Electronic Structure (ES) and Molecular Dynamics (MD) training workshop that began in October 2021. The focus is to train African researchers in ML and its application in ES and MD.

Directors:

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G-M. Rignanesse (UCL, Belgium)
M. Scheffler (Fritz-Haber MPG, Germany)

Local Organisers:

O. Akin-Ojo (ICTP-EAIFR & Univ. Rwanda)
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Description:

A recap of the Python language, ML and Materials Databases will be made. This will be quickly followed by joint projects in materials discovery. Each day will feature hands on training sessions as well as two to three talks from experts in the field presenting their research.

Topics:

- Introduction to the Python language
- Introduction to Machine Learning
- Databases for Materials Discovery
- Machine Learning for force fields development for
- Molecular Dynamics Simulations
- Machine Learning in Electronic Structure

ICTP Scientific Contact:

A. Hassanali (ICTP, Trieste, Italy)

Speakers:

O. Akin-Ojo (ICTP-EAIFR & Univ. Rwanda)
J. Behler (Univ. Göttingen, Germany)
M. Ceriotti (EPFL, Switzerland)
B. Cheng (IST, Austria)
G. Csanyi (Univ. Cambridge, U.K.)
S. Cutarolo (Duke Univ. U.S.A.)
S. de Gironcolli (SISSA, Trieste, Italy)
A. Jain (LBNL, USA)
E. Kucukbenli (Boston Univ., USA)
A. Laio (SISSA, Italy)
M. Parrinello (ETH, Zurich)
G-M. Rignanesse (UCL, Belgium)
M. Scheffler (Fritz-Haber MPG, Germany)
Y. Shaidu (UC Berkely, U.S.A.)

How to apply:

Online application:
<http://indico.ictp.it/event/9787/>

Female scientists are encouraged to apply.

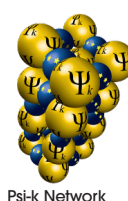
Priority will be given to those who actively participated in the ML training from October 2021.

Grants:

There is no registration fee.

Deadline:

15 April 2022



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