



Current Opinion in Structural Biology

Biophysics School on Integrated Machine Learning and QM/MM Molecular Dynamics Simulations in Understanding Biological Systems & Cell Machinery

21 Sept – 1 Oct, 2021

University of Dodoma (UDOM), Dodoma, Tanzania.

Understanding the chemical interactions and molecular machinery of biological systems is an important step towards designing bio-inspired materials. However, understanding specific and nonspecific interactions in nature at the molecular scale are limited. Molecular dynamics (MD) simulations provide a means to study biophysical systems with atomistic details. Machine learning (ML) on other hand, provide a means to synthesize meaningful insights from the deluge of high-dimensional data generated by MD. In this school participants will be introduced to the concept and ideas of ML and MD and how the two can be coupled to yield insights on the molecular interactions towards designing drug.

TOPICS:

QM/MM Molecular dynamics, Free energies, Machine Learning, Numerical methods, Nanoscience, Biophysics, Data Sciences.

Application: click [here](#)

Inquiries email to:

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Funding

Limited funding is available to cover transport, meals and accommodation.

Female applicants are encouraged to apply.

Deadline is 15 August 2021

Directors

D.M. Shadrack (SJUT, Tanzania)

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Organizers

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Speakers/Lecturers

E. Menkah (Ghana)

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E. Roldan (ICTP, ITALY) and many more...

