



THE HONG KONG UNIVERSITY OF SCIENCE & TECHNOLOGY

Department of Mathematics

## PHD STUDENT SEMINAR

# Learning Molecular Dynamics with LSTM and Transformer

By

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### Abstract

Recurrent neural networks like long short-term memory (LSTM) have been utilized as a tool for modeling and predicting dynamics of complex stochastic molecular systems. Previous studies have shown that Transformer has an advantage over LSTM in dealing with the memory loss of long-sequence data, and exceeds LSTM in many natural language processing tasks. In this seminar, we will show the implementation of Transformer on learning molecular dynamics and compare it with LSTM, which is greatly affected by lag time.

**Date : 3 May 2021 (Monday)**

**Time : 3:00pm**

**Zoom Meeting : <https://hkust.zoom.com.cn/j/6218914432> (Passcode: hkust)**

*All are Welcome!*