國立中山大學應用數學系
學術演講

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講　題：Molecular transport and reactivity in nanoporous materials, and RNA secondary structure prediction.

時　間：2023/05/04（Thursday）14:10 ~ 15:00

地　點：理 SC 4009-1 教室 (視訊並行)

茶　會：13:30

Google Meet Link：https://meet.google.com/evg-ukyx-opd

Abstract

In the first half hour, we will introduce the inhibited passing of reactant and product molecules within the linear pores of nanoporous catalytic materials strongly reduces reactivity. The dependence of the passing propensity P on pore radius R is analyzed utilizing Langevin dynamics to account for solvent effects. Our analysis shows that P~(R−Rc)^σ, where passing is sterically blocked for R ≤ Rc, with σ below the transition state theory value. Deeper insight comes from analysis of the corresponding high-dimensional Fokker-Planck equation, which facilitates an effective small-P approximation, and dimensional reduction enabling utilization of conformal mapping ideas. We analyze passing for spherical molecules and also assess the effect of rotational degrees of freedom for elongated molecules.

The remaining part of this talk will focus on the application of machine learning on RNA secondary structure. Our research applies the combinations of machine learning methods to predict RNA secondary structure through Neural Network, Random Forest, Extreme Gradient Boosting (XGBoosting), LightGBM (Light Gradient Boosting Machine,LGBM), etc. The F1-score we obtained is around 0.914, which is better than traditional prediction methods, but the newer deep learning methods still perform (F1-score 0.937) better than us.

敬 請 公 告！ 歡 迎 參 加！

應用數學系：http://math.nsysu.edu.tw

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