

**The Hong Kong Polytechnic University  
Department of Applied Mathematics**

**Colloquium**

**Unitary Algorithm**

**By**

**Prof. Aihui ZHOU  
Academy of Mathematics and Systems Science  
Chinese Academy of Sciences**

**Abstract**

To obtain convergent numerical approximations without using any orthogonalization operation is of great importance in electronic structure calculations. In this presentation, we introduce a class of iteration schemes for the discretized Kohn-Sham Density Functional The iterative approximations are guaranteed to converge to the Kohn-Sham orbit any orthogonalization when the initial orbitals are orthogonal.



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**Date: 11 March 2022 (Thursday)**

**Time: 10:00-11:00 (Hong Kong Standard Time GMT +8)**

**Venue: Online Talk via Zoom (Meeting ID: 917 1897 4374)**

**Speaker: Prof. Aihui Zhou, Academy of Mathematics and Systems Science,  
Chinese Academy of Sciences**

**Host: Prof. Zhonghua Qiao, The Hong Kong Polytechnic University**

**Click to join:**

**<https://polyu.zoom.us/j/91718974374?pwd=YTRjZzlMaWZRLzZwNktBN0Z5LzNZUT09>**

**\*\*\* ALL ARE WELCOME \*\*\***

For enrolment, please send your name and email to [wai-yan.moon@polyu.edu.hk](mailto:wai-yan.moon@polyu.edu.hk) on or before 10 March 2022