



## Colloquium

Department of Engineering and  
System Science,  
Institute of Nuclear Engineering  
and Science,  
National Tsing Hua University

### Surface Defects as Catalysts: DFT Analysis of Enhanced Reactivity in $\text{PtTe}_2$

**In this talk, the following content  
will be presented:**

The study enhances  $\text{PtTe}_2$ 's efficiency in decomposing methanol by creating surface defects, particularly under-coordinated Pt sites at Te vacancies. Through the integration of density functional theory (DFT) calculations and experimental validation, it is shown that these defects markedly boost the catalytic performance, facilitating the conversion of methanol into diverse products. This research underscores the potential of merging surface defect engineering with DFT insights to refine catalysts, representing a notable progress in the field of catalysis.



周至品教授

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#### Experience:

- **2023~now** Associate Professor, Department of Physics, National Changhua University of Education, Taiwan
- **2020~2023** Assistant Professor, Department of Physics, National Changhua University of Education, Taiwan
- **2017~2020** Research Fellow, Department of Mechanical Engineering, City University of Hong Kong, Hong Kong SAR.
- **2013~2017** Postdoctoral Research Fellow, Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Hungary.
- **2009~2013** Postdoctoral Research Fellow, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan.

**15:30-17:00, Wednesday, March 13th, 2024**

**NE69 ESS Building, NTHU**

**101, Sec. 2, Kuang-Fu Rd., Hsinchu 300044, Taiwan**