

國立中央大學數學系

專題演講

主 講 人：胡全榮教授 (新加坡南洋理工大學)

演講題目：Periodic topology on solar cell material analysis

演講茶會：2023年11月09日(星期四) 3:30 p.m. ~ 4:00 p.m.

茶會地點：中央大學鴻經館M306

演講時間：2023年11月09日(星期四) 4:00 p.m. ~ 5:00 p.m.

演講地點：中央大學鴻經館M107

Abstract：

With its extraordinary efficiency, cost-effectiveness, and impressive stability, 2D perovskite holds immense promise for transforming photovoltaic technology, particularly in solar cell development. However, the limitations of current material structure representations have significantly impeded AI-based perovskite design and discovery. In this presentation, we introduce a novel framework that integrates topological data analysis (TDA), periodic geometry, and machine learning to effectively represent 2D perovskite structures and predict their bandgaps. This innovative approach enables the detection of the inherent periodic geometry and topology within the material's atomic system, surpassing the traditional focus on chemical interactions among atoms and unit cell periodicity. We employ mathematical tools such as persistent homology, quotient complexes, and density fingerprints to encode this essential periodicity in the topological and geometric aspects of the crystalline structure. Additionally, we provide a comprehensive and concise introduction to these tools in the context of TDA and periodic geometry.

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