應用力學所專題討論公告

IAM Seminar Announcement

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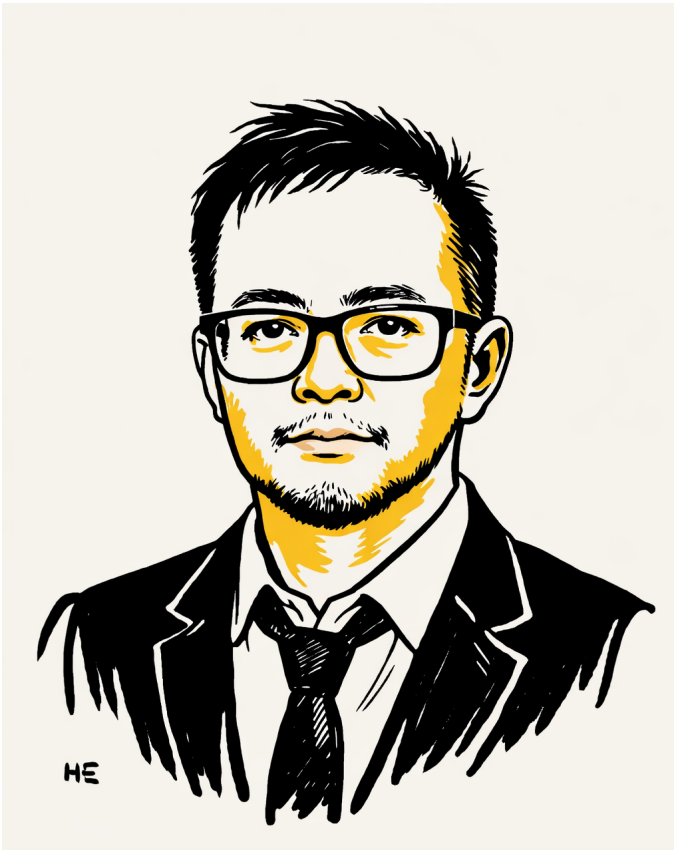
講　題：分子吸附對二維材料電性調控之第一性原理研究
主持人：張建成教授
日　期：115年4月13日(星期一)
時　間：下午2時20分
地　點：台灣大學應用力學研究所國際會議廳



分子吸附對二維材料電性調控之第一性原理研究

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摘要

二維過渡金屬二硫族化物（TMDs）因具備優異的尺寸縮放潛力與可調控的電子性質，被視為下一世代電子元件的重要候選材料。然而，在這類原子級薄材料中實現可控制且不破壞結構的摻雜，仍然是一項關鍵挑戰。 本演講將介紹我們近期在「非破壞性分子摻雜」上的研究成果。透過第一原理計算，我們展示不同有機分子如何透過電荷給予或吸引，有效調控如 WSe2 與 MoS2 的載子型態與功函數，同時維持其原有晶格結構。 此外，我們進一步探討缺陷與外加電場對摻雜行為的影響。結果顯示，材料中的缺陷會顯著改變電荷轉移效率，而外加電場（可類比為電晶體閘極效應）則提供額外的調控手段。這些現象可從界面電荷重分佈以及費米能階附近分子態的形成來理解。 本研究提供一個清楚的物理圖像，說明如何透過分子與材料界面的交互作用，實現可調控且可逆的摻雜機制，並對未來奈米電子元件設計提供重要啟發。

Two-dimensional (2D) transition metal dichalcogenides (TMDs) have emerged as promising materials for next-generation electronic devices due to their excellent scalability and tunable electronic properties. However, achieving controllable doping in these atomically thin systems remains a critical challenge, as conventional approaches often introduce structural damage. In this talk, I will present our recent work on non-destructive molecular doping as an alternative strategy to engineer the electronic properties of TMDs such as WSe2 and MoS2. Using first-principles calculations, we demonstrate how different organic molecules can effectively donate or withdraw charge, leading to significant modulation of carrier type and work function without disrupting the lattice structure. I will further show that the doping behavior is strongly influenced by both intrinsic defects and external electric fields. In particular, defects can enhance or suppress charge transfer, while an applied electric field—mimicking transistor gating—provides an additional degree of control over the electronic structure. These effects can be understood through interfacial charge redistribution and the emergence of molecular states near the Fermi level. This work provides a physical picture of how molecule–surface interactions can be harnessed to achieve tunable and reversible doping in 2D materials, offering practical insights for future nanoelectronic device design.