

From Material Structure to Device Function: Porous Coordination Frameworks at Semiconductor Interfaces for Gas Sensors and Solar Cells

從材料結構到元件功能：多孔配位框架－半導體界面於氣 體感測器與太陽能電池之應用

English Abstract:

Porous coordination frameworks, including metal-organic frameworks (MOFs) and coordination polymers (CPs), offer molecular-level tunability of pore size, ligand electronic structure, and optical response. However, the organic ligands and coordination bonds that confer these functions also limit their thermal stability and hinder their integration into conventional semiconductor devices. This talk presents an approach for translating material structure into device function, in which device behavior is predicted from structural parameters and the dominant mechanism behind performance changes is identified through control experiments. Two case studies illustrate this approach: a ZIF-8 molecular sieving membrane on amorphous InGaZnO (a-IGZO) gas sensors, where the pore aperture confers hydrogen selectivity and UV activation, in place of thermal activation, preserves long-term stability; and a luminescent zinc phosphate CP overlayer on textured silicon solar cells, where the efficiency gain is attributed to spectral downconversion. These studies show that systematically correlating material characteristics with device performance provides a rational basis for integrating porous coordination frameworks into semiconductor devices.

中文摘要：

多孔配位框架（包含金屬有機框架與配位聚合物）可於分子層級調控孔徑尺寸、配體電子結構與光學響應。然而，賦予其功能的有機配體與配位鍵結，同時限制了材料的熱穩定性，使其難以整合於傳統半導

體元件。本演講介紹一套從材料結構到元件功能的轉譯方法：由框架的結構參數預測元件的功能，並透過對照實驗，釐清元件性能變化的主導機制。演講以兩個案例說明此方法：其一是將 ZIF-8 分子篩選膜整合於非晶銦鎵鋅氧化物 (a-IGZO) 氣體感測器，利用孔徑賦予氫氣選擇性，並以紫外光活化取代熱活化，維持元件的長期穩定性；其二是將發光型鋅磷酸鹽配位聚合物塗佈於纖維化矽太陽能電池表面，並釐清其效率提升來自光譜下轉換。上述結果顯示，系統性地建立材料特性與元件性能之間的關聯，可為多孔配位框架整合於半導體元件提供合理的設計依據。