**Photocatalytic CO2 reduction and excited state carrier dynamics**

Photocatalysis technology is considered as an effective way to alleviate energy crisis and environmental pollution. However, the low energy conversion efficiency has become the main factor restricting its practical application. Improving the electron-hole separation efficiency and clarifying the dynamic process of excited carrier constitute an urgent goal. Base on the density functional theory (DFT) and nonadiabatic molecular dynamics (NAMD) method, we investigate the relationship between the ferroelectric polarization and electronic properties and excited state dynamics. Our study uncovers the carrier dynamics images in CuBiP2Se6 systems and proposes a novel approach for high activity and selectivity of photocatalytic CO2 reduction based on ferroelectric polarization. These findings provide valuable fundamental insights for the development and design of novel photocatalysts.