

Single-atom catalyst

- ❑ DFT model (Figs. 1-1 & 1-2) as the guide for the structural system development;
- ❑ Structural system is developed with the element coordination environment progressively fine-tuned to search for the unknown local structure adjustment when the site occupancy occurred;
- ❑ XANES theoretical spectrum system (Fig. 1-3) based on the developed structure system.

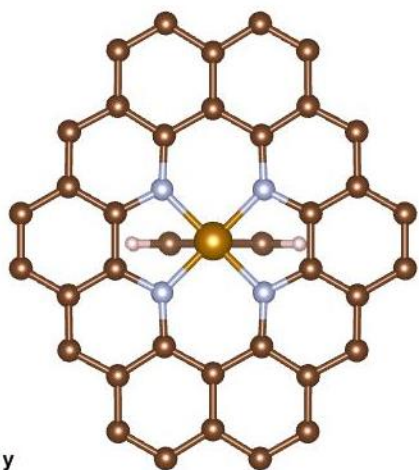


Fig.1-1

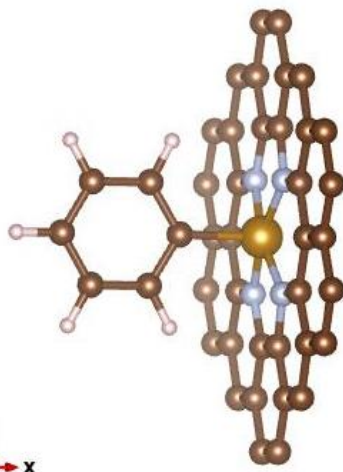


Fig.1-2

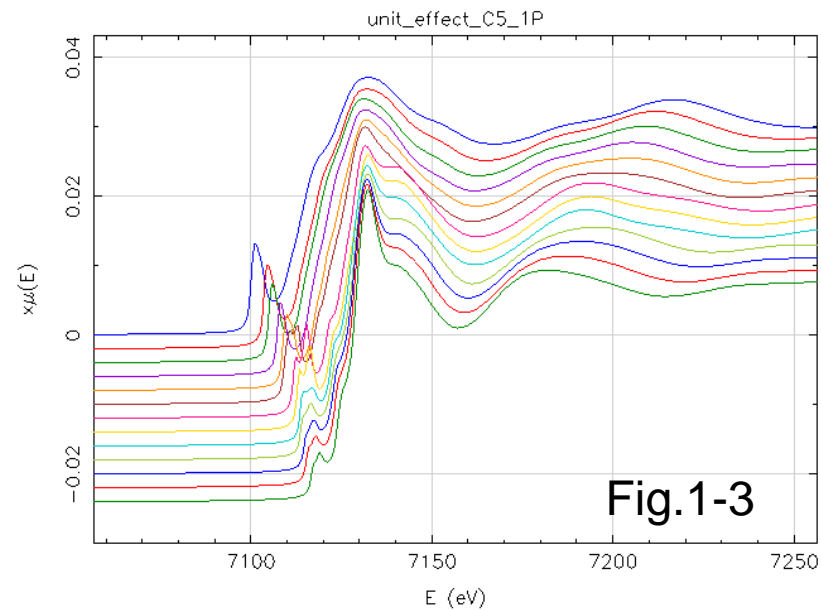


Fig.1-3