

Element Site Occupancy in Crystalline Material

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

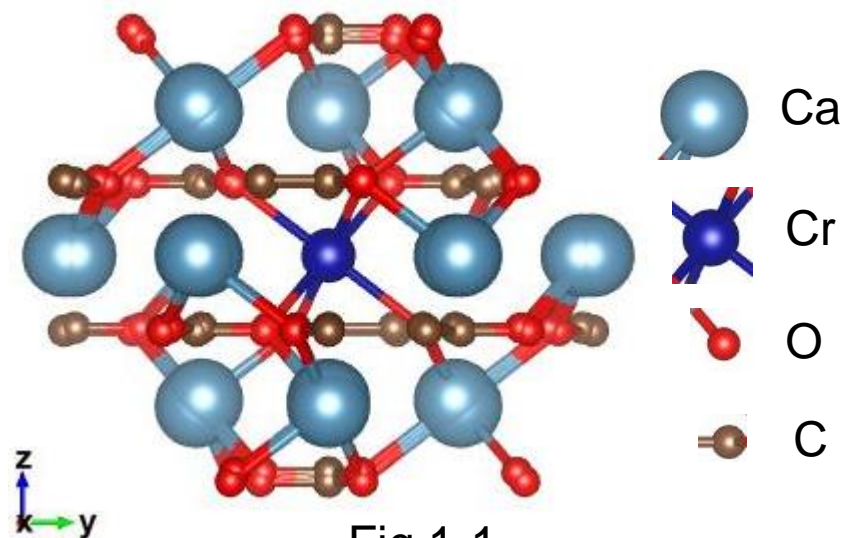


Fig.1-1

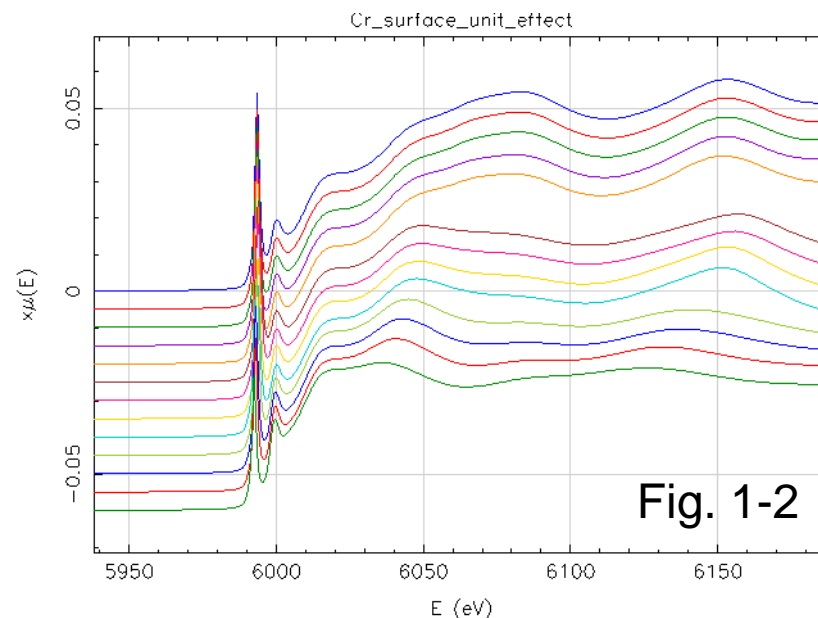


Fig. 1-2