

# Element Surface Site Occupancy

- ❑ 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 (Figs 1-1 & 1-2);
- ❑ XANES theoretical spectrum system (Fig. 1-3) based on the developed structure system.

