DFT & AIMD Simulations with VASP for Energy Systems

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Training Program

Introduction

- **Overview of energy systems:** batteries, SOECs, fuel cells, ammonia production
- **Importance of DFT** for mechanistic insights
- **Role of AIMD** for instantaneous events and short-timescale dynamics

VASP Basics

- **Key input/output files:**
  - POSCAR, INCAR, KPOINTS, POTCAR
- **Setting up calculations:**
  - Structural relaxation
- **Important parameters** for convergence

DFT for Mechanistic Insights

- **Geometry optimization:** structures of materials and adsorbates
- **Adsorption energies and reaction barriers:** identifying stable states and transition states
- **Demonstration:** oxygen adsorption on a surface
- **Thermal corrections:** accounting for temperature effects (e.g., from 0 K to 300 K)

AIMD for Instantaneous Events

- **AIMD setup in VASP:** NVT and NPT ensembles
- **Observing short-timescale dynamics:** bond breaking, diffusion
- **Demonstration:** small system at finite temperature

Hands-On Mini Exercise

- **Set up a small system** in VASP (e.g., AO on PE or catalytic site)
- **Run:**
  - Geometry optimization + short AIMD (~100–200 fs)
- **Visualize results:** folding, bond breaking, dynamics

Wrap-Up & Discussion

- **Key takeaways:** when to use DFT vs AIMD
- **Limitations** and tips for larger systems
- **Q&A** and next steps