Vacancy Defects in Double Transition Metal MXenes

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Motivation

Double Transition Metal (DTM) MXenes

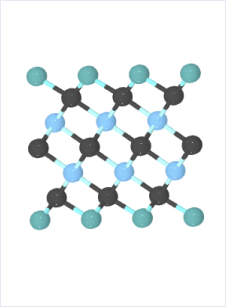

Figure 1: $Mo_2Nb_2C_3$ MXene

Vacancy Defects

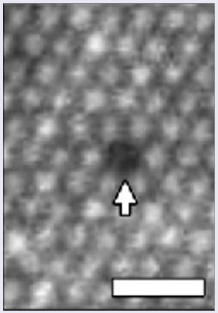

Figure 2: Vacancy defect in Ti_3C_2X MXene [1]

Research Question

How do vacancy defects affect the stability and electronic properties of double transition metal MXenes?

Simulation Details

DFT Parameters

- Exchange-correlation functional: PBE
- Pseudopotential: PAW
- Energy cutoff: 40 Ry $\rightarrow$ 520 eV
- k-point grid: $6 \times 6 \times 1$

Running DFT

- QuantumESPRESSO 7.1
- nanoHUB / Negishi
- *pymatgen* to generate input files
- Example code at `https://github.com/katnykiel/mxene-point-defects-workflow.git`

Input Script

```
# Create a cell relaxation sim
make_sim(
    name,
    struct,
    control={
        "pseudo_dir": "./pseudo/pseudo_PAW/",
        "calculation": "vc-relax",
        "outdir": "./",
        "tstress": True,
    },
    system={"ecutwfc": 40, "nosym": True},
    cell={"cell_dofree": "fixc"},
    kpoints_grid=[6, 6, 1],
)

# Run relax simulation
run_sim(name, struct)
```

Figure 3: Sample input script code

Convergence Testing

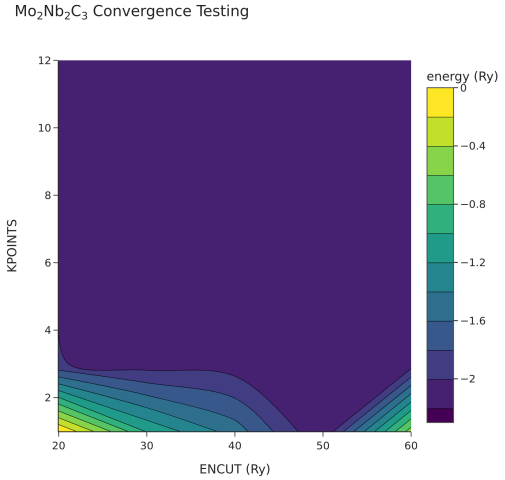

Figure 4: DFT hyperparameter convergence

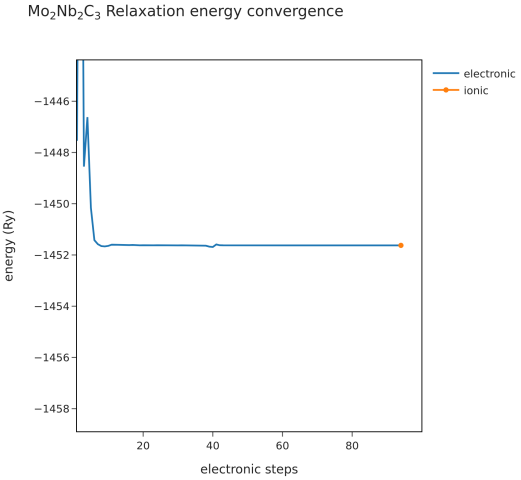

Figure 5: Cell relaxation energy convergence

Calculating Vacancy Energy

Formation Energy

$$E_{\text{form}}^{MXene} = E^{MXene} - \sum_{i=\{M,X\}} N_i * \left(\frac{E_i^0}{n_i^0}\right)$$

- E^{MXene}: energy of MXene cell
- N_i: number of atoms of type i in MXene supercell
- E_i^0: energy of atom i in its equilibrium phase
- n_i^0: number of atoms of type i in equilibrium phase

Simulation

- Calculate the energy of the perfect MXene
- Calculate the energy of the MXene with a vacancy defect
  - Before relaxation
  - After relaxation
- Calculate the energies of each component phase