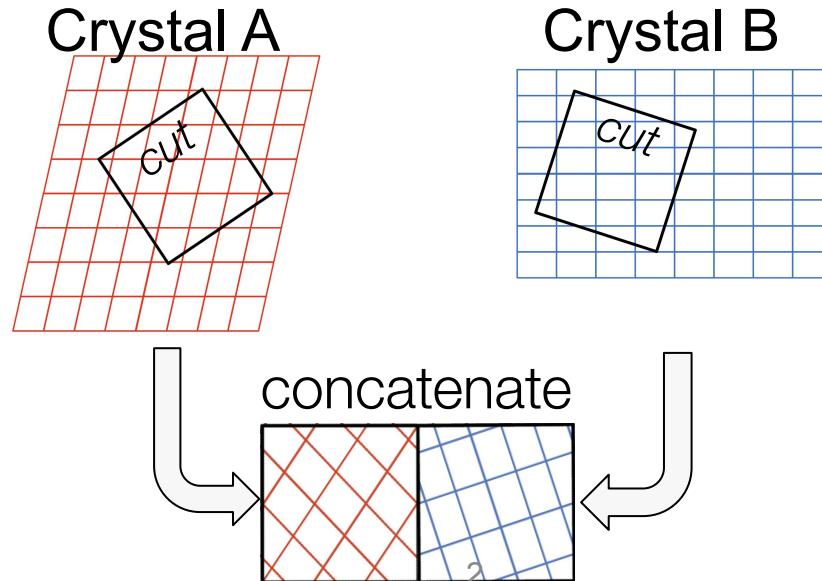


Results: Ni / TiO₂ interface

Model training

- Crystal structures
 - Anatase TiO₂: mp-390
 - Ni: mp-23
- Interface structure generation: cut-concatenate method



Model training

- Initial dataset
 - 10 random interface structures + crystal Ni & TiO₂
 - MD sampling
- Active learning
 - 10 iterations
 - Script
 - Temperature 500~2000K
 - NVT, 2ps
 - NPT, 15-30 ps
 - NVT at 500K higher T, 5-10 ps
- Final training:
 - Both small / large models

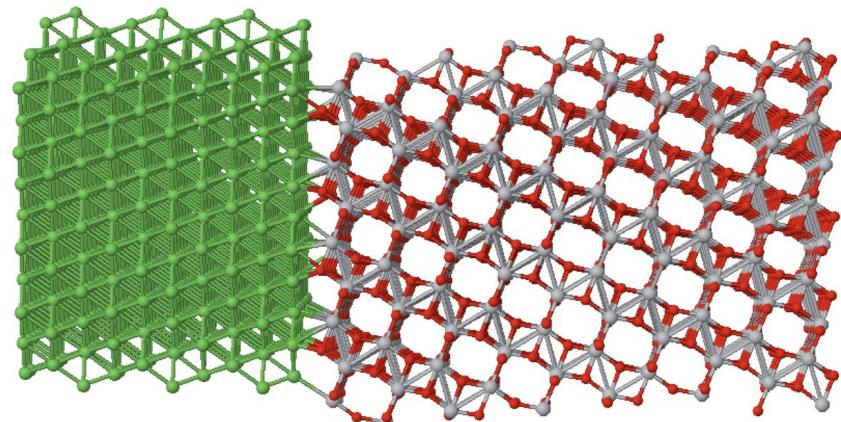
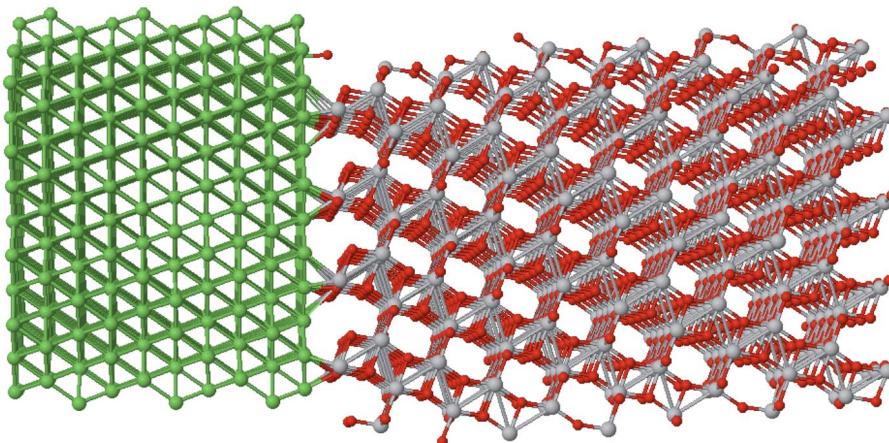
Evaluation

- Evaluation structures
 - 6 Interface structures
 - Ni (111) / TiO₂ (101) interface (Ti / O terminations)
 - Ni (110) / TiO₂ (001) interface (Ti / O terminations)
 - Ni (100) / TiO₂ (001) interface (Ti / O terminations)
- MD simulations with PFP/LightPFP
 - NVT 5ps + NPT 100 ps
 - Temperatures: 1200K, 1400K and 1600K
- Models
 - Small/Large models

Evaluation

Ni (111) / TiO₂ (101) interface

- Generated by pymatgen with low lattice strain.
- There are two termination types for TiO₂ slab

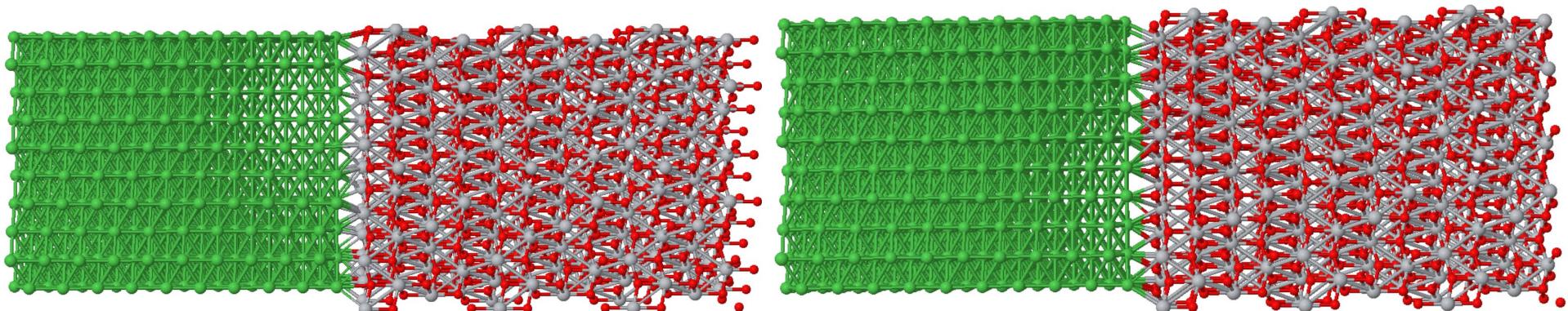


Ni (111) / TiO₂ (101) interface structures; (left) Ti termination, (right) O termination

Evaluation

Ni (110) / TiO₂ (001) interface

- Generated by pymatgen with low lattice strain.
- There are two termination types for TiO₂ slab

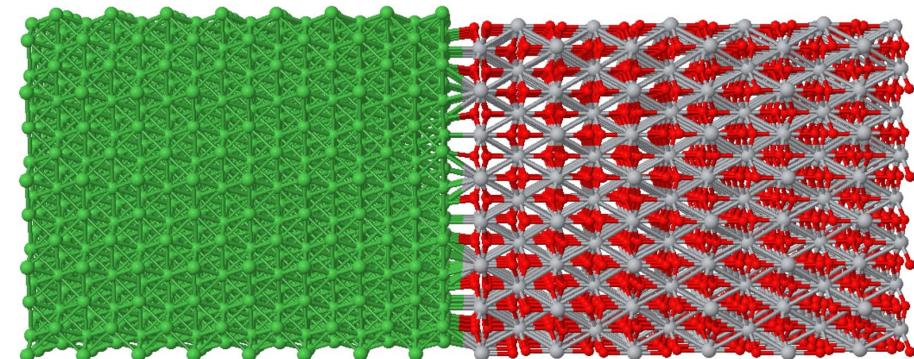
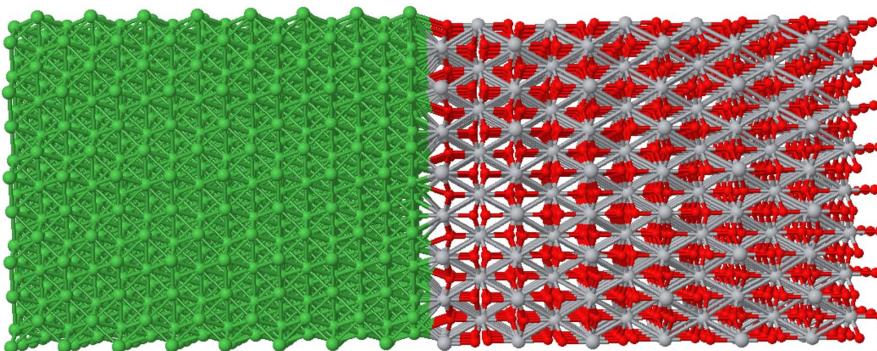


Ni (110) / TiO₂ (001) interface structures; (left) Ti termination, (right) O termination

Evaluation

Ni (100) / TiO₂ (001) interface

- Generated by pymatgen with low lattice strain.
- There are two termination types for TiO₂ slab



Ni (100) / TiO₂ (001) interface structures; (left) Ti termination, (right) O termination

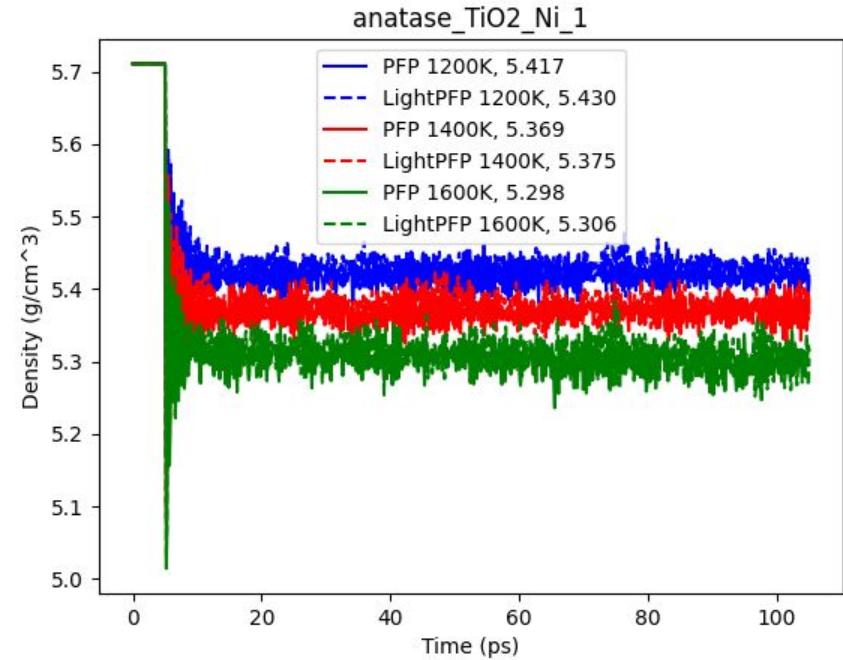
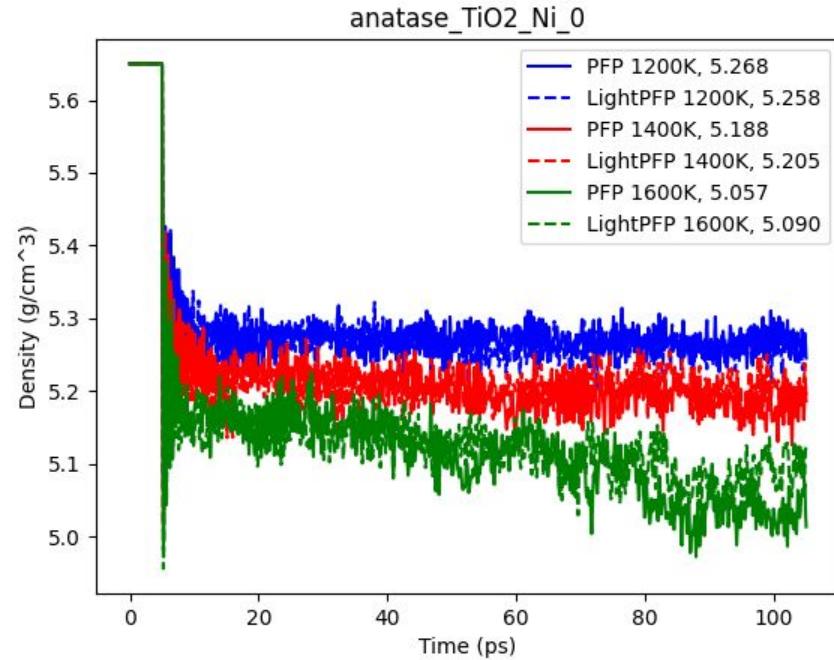
Evaluation: Density

Density

	Temperature	Density (g/cm3)			Density error (g/cm3)	
		PFP	LightPFP small	LightPFP Large	LightPFP small	LightPFP Large
Ni (111) / TiO2 (101) interface (Ti terminations)	1200K	5.268	5.258	5.269	0.01	0.001
	1400K	5.188	5.205	5.178	0.017	0.01
	1600K	5.057	5.09	5.041	0.033	0.016
Ni (111) / TiO2 (101) interface (O terminations)	1200K	5.417	5.43	5.44	0.013	0.023
	1400K	5.369	5.375	5.391	0.006	0.022
	1600K	5.298	5.306	5.331	0.008	0.033
Ni (110) / TiO2 (001) interface (Ti terminations)	1200K	5.77	5.763	5.778	0.007	0.008
	1400K	5.677	5.67	5.685	0.007	0.008
	1600K	5.414	5.333	5.485	0.081	0.071
Ni (110) / TiO2 (001) interface (O terminations)	1200K	5.828	5.835	5.852	0.007	0.024
	1400K	5.77	5.772	5.795	0.002	0.025
	1600K	5.68	5.659	5.693	0.021	0.013
Ni (100) / TiO2 (001) interface (Ti terminations)	1200K	5.971	5.974	5.985	0.003	0.014
	1400K	5.871	5.88	5.908	0.009	0.037
	1600K	5.584	5.478	5.398	0.106	0.186
Ni (100) / TiO2 (001) interface (O terminations)	1200K	6.061	6.088	6.106	0.027	0.045
	1400K	5.992	5.992	6.034	0	0.042
	1600K	5.878	5.858	5.926	0.02	0.048
		9			0.0209	0.0348

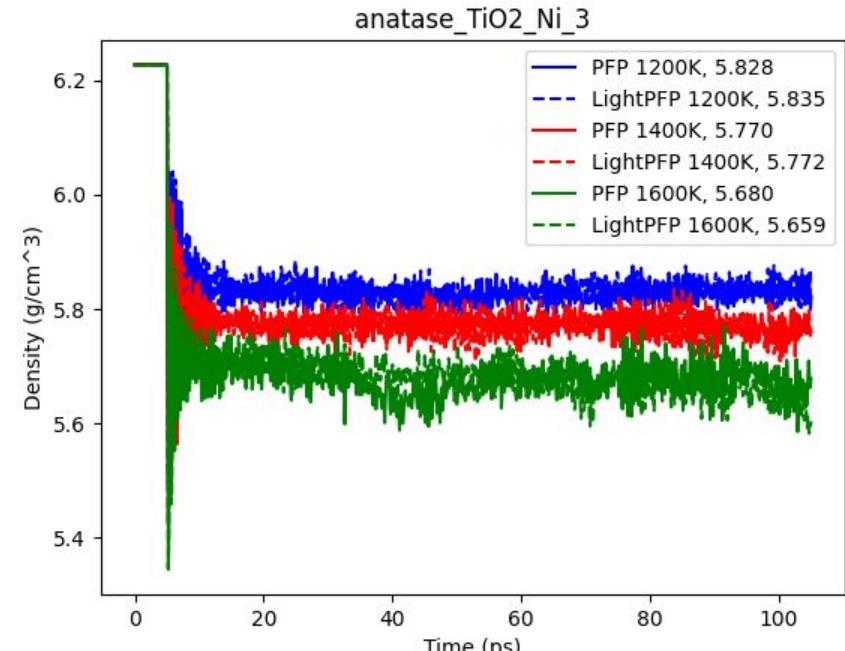
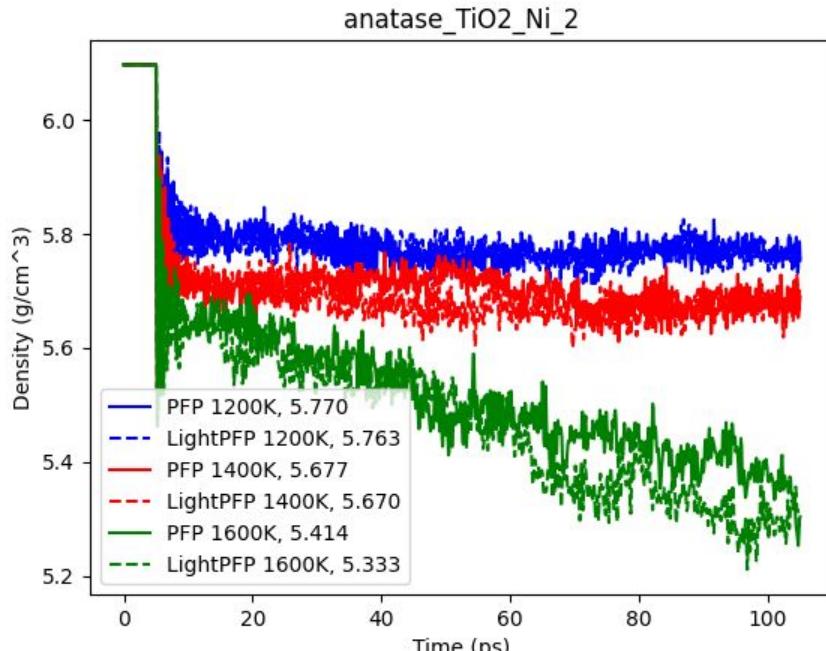
Density: Small model; Ni (111) / TiO₂ (101) interface (Ti / O terminations)

- Density
 - Small model
 - Ni (111) / TiO₂ (101) interface (Ti / O terminations)



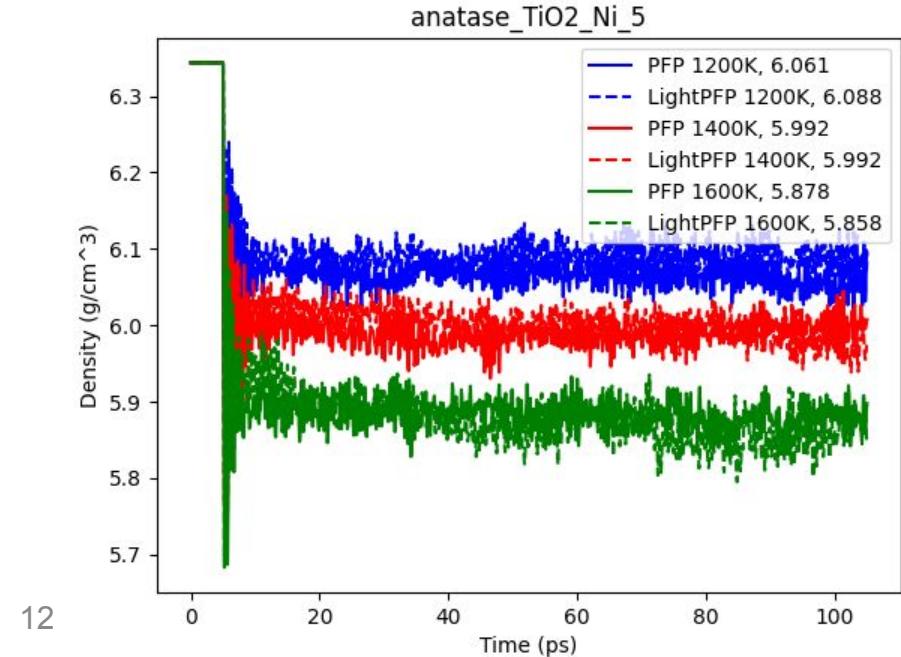
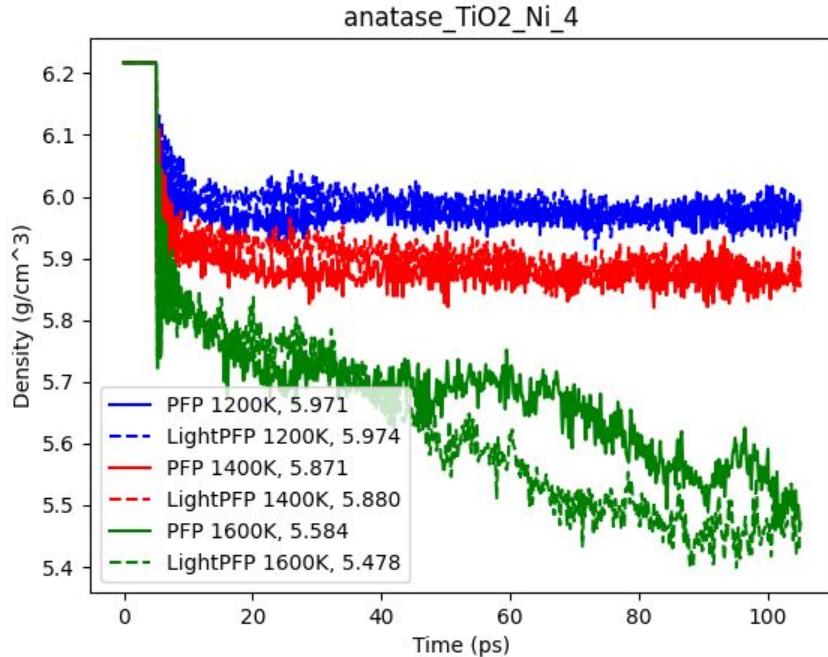
Density: Small model; Ni (110) / TiO₂ (001) interface (Ti / O terminations)

- Density
 - Small model
 - Ni (110) / TiO₂ (001) interface (Ti / O terminations)



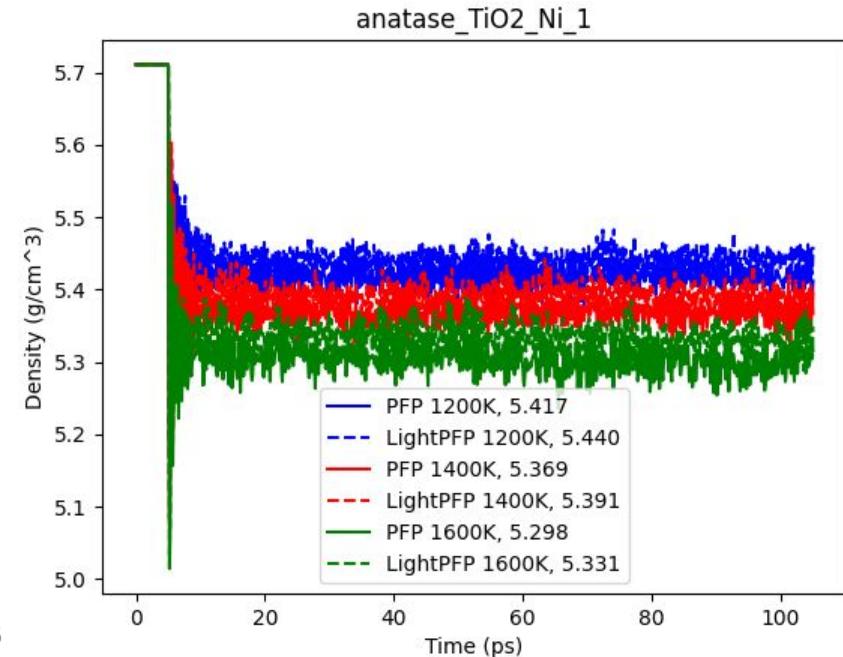
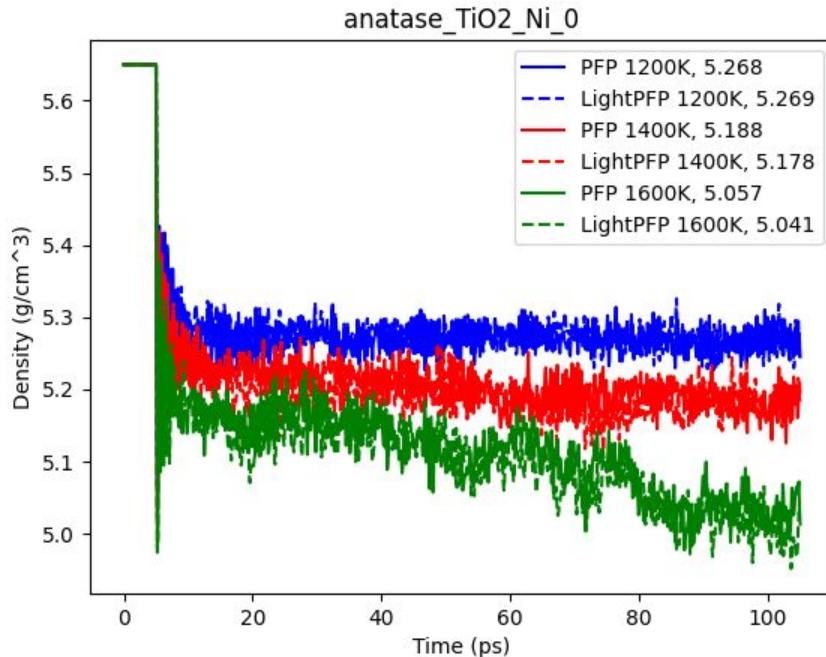
Density: Small model; Ni (100) / TiO₂ (001) interface (Ti / O terminations)

- Density
 - Small model
 - Ni (100) / TiO₂ (001) interface (Ti / O terminations)



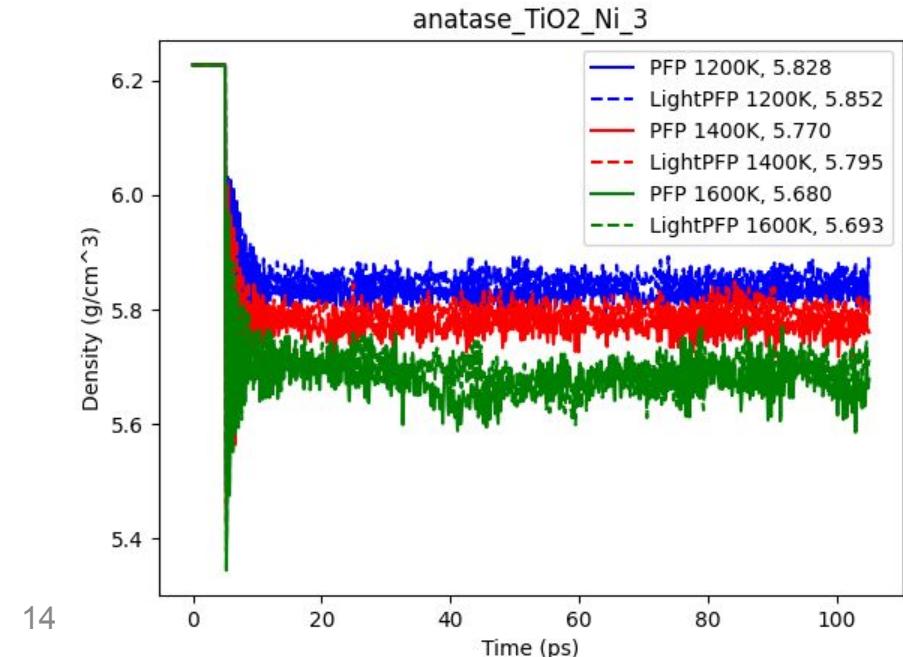
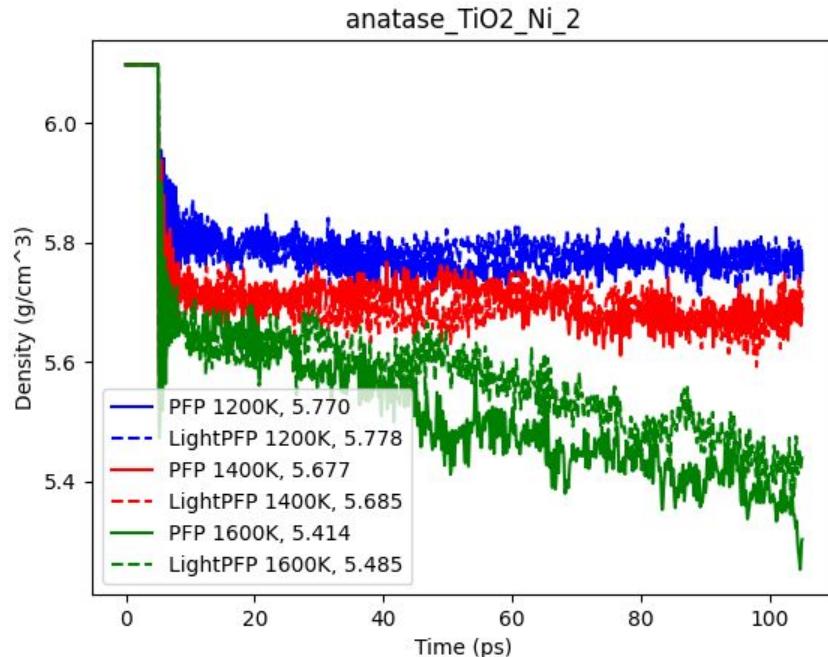
Density: Large model; Ni (111) / TiO₂ (101) interface (Ti / O terminations)

- Density
 - Large model
 - Ni (111) / TiO₂ (101) interface (Ti / O terminations)



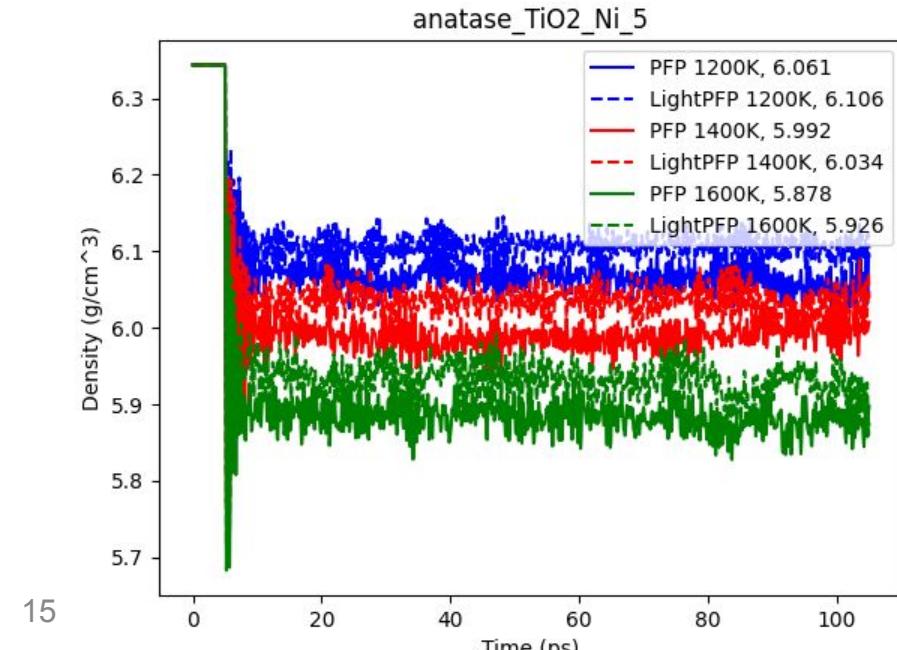
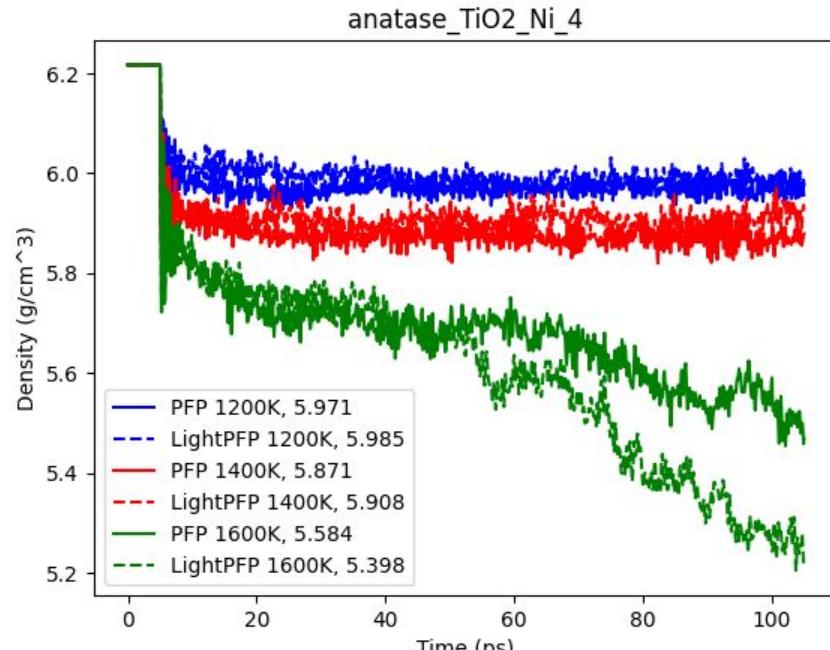
Density: Large model; Ni (110) / TiO₂ (001) interface (Ti / O terminations)

- Density
 - Large model
 - Ni (110) / TiO₂ (001) interface (Ti / O terminations)



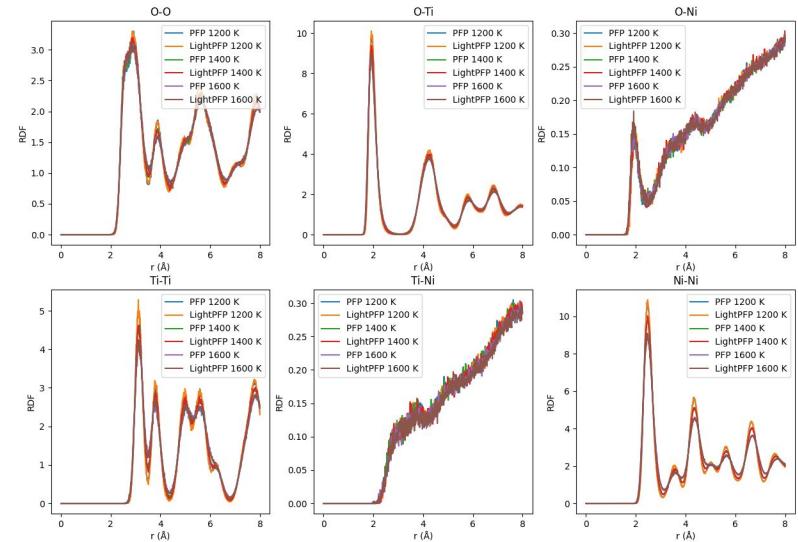
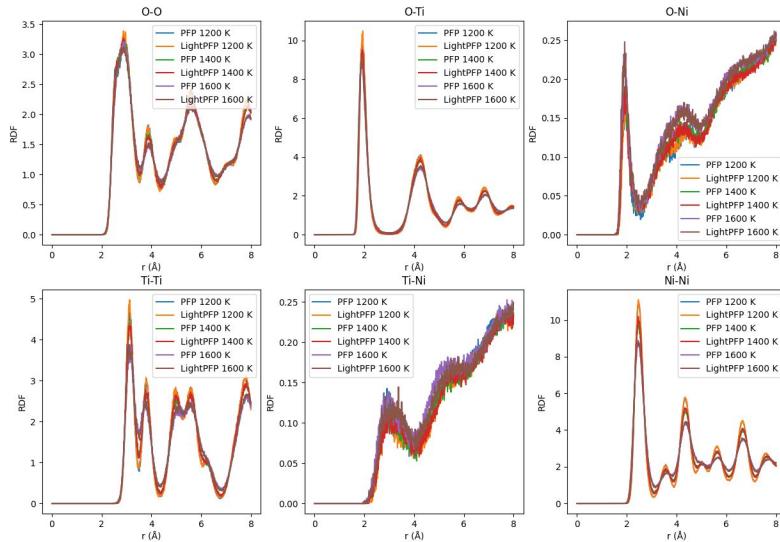
Density: Large model; Ni (100) / TiO₂ (001) interface (Ti / O terminations)

- Density
 - Large model
 - Ni (100) / TiO₂ (001) interface (Ti / O terminations)

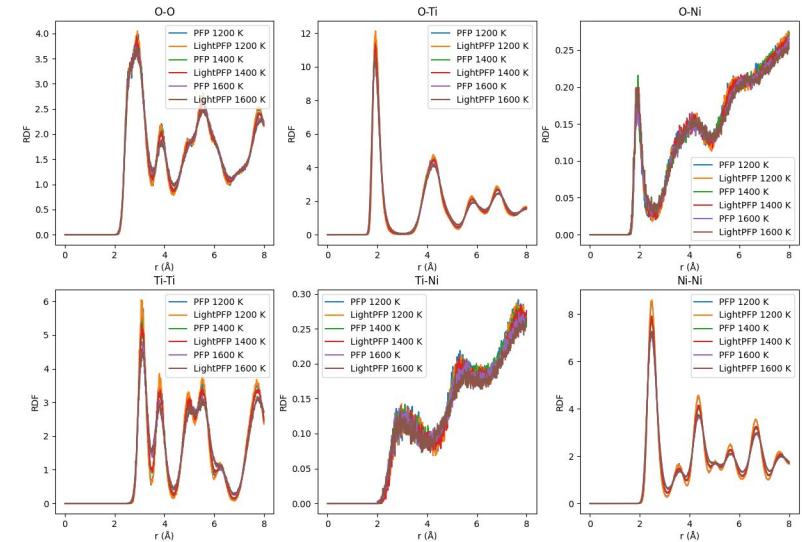
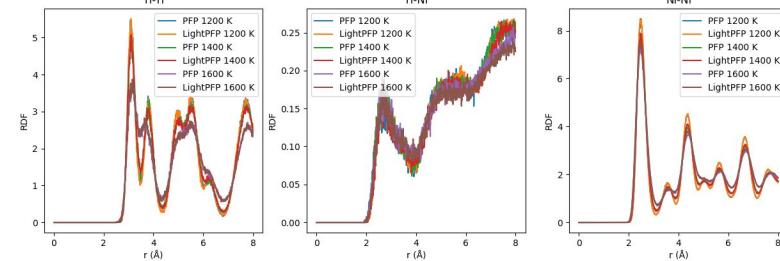
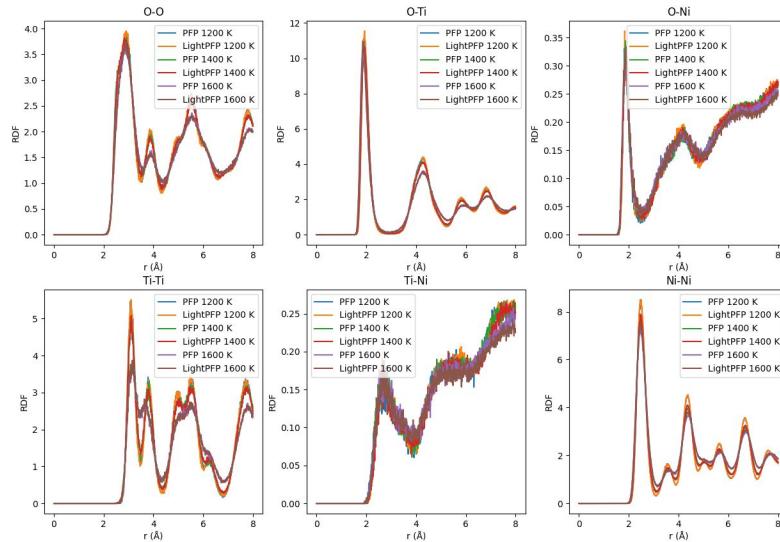


Evaluation: RDF

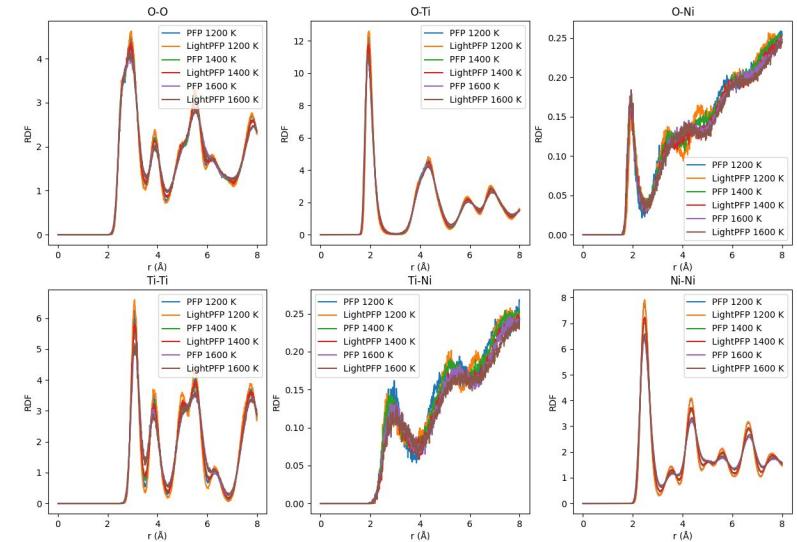
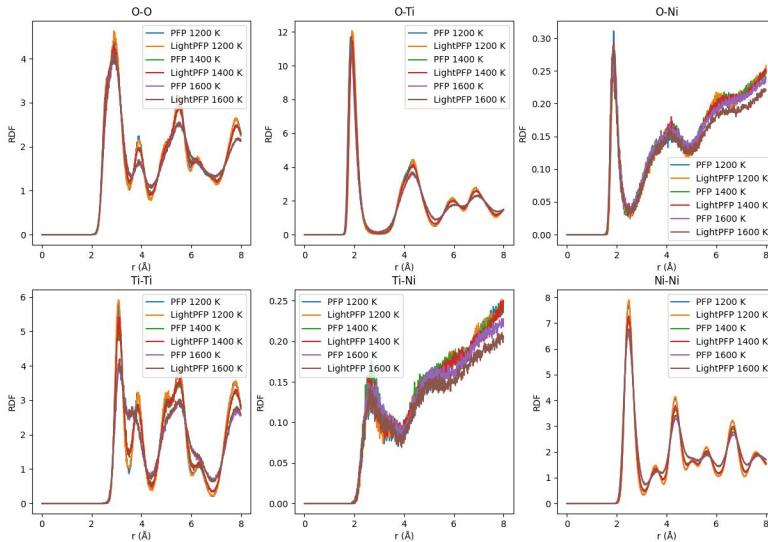
RDF: Small model; Ni (111) / TiO₂ (101) interface (Ti / O terminations)



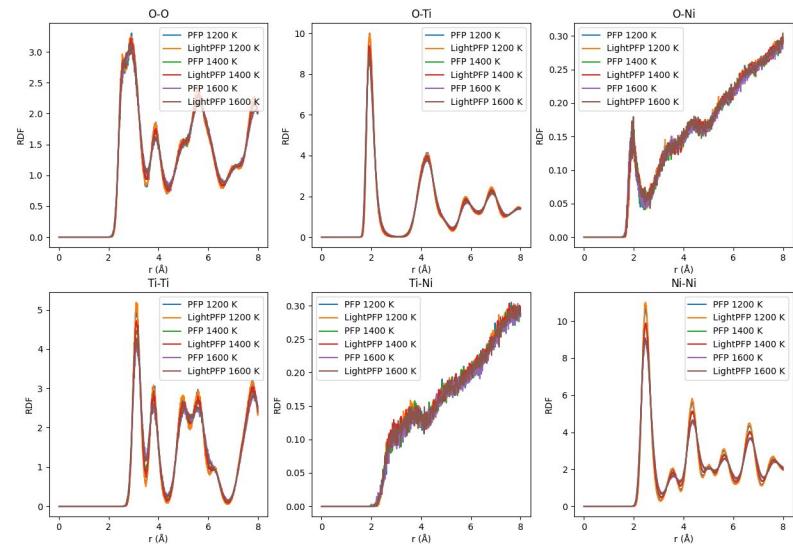
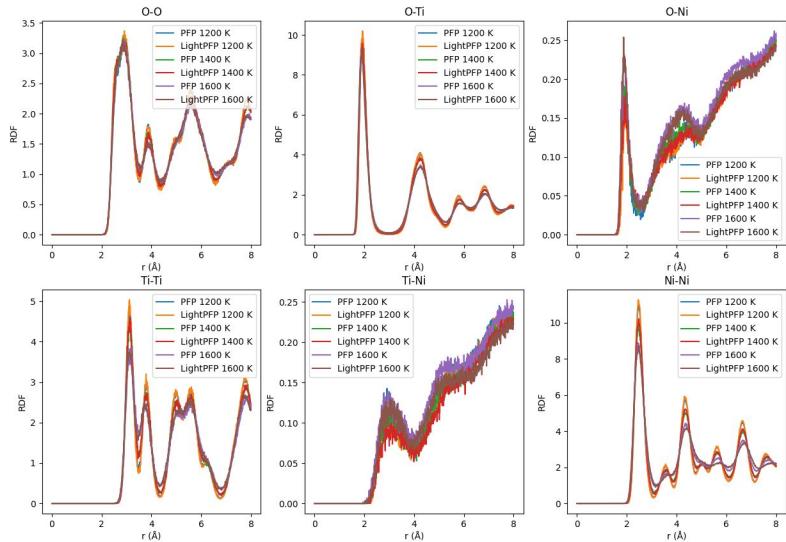
RDF: Small model; Ni (110) / TiO₂ (001) interface (Ti / O terminations)



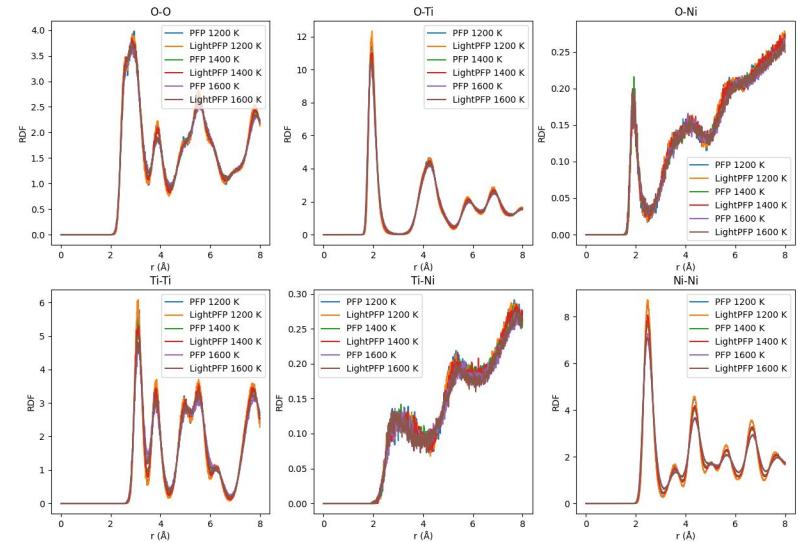
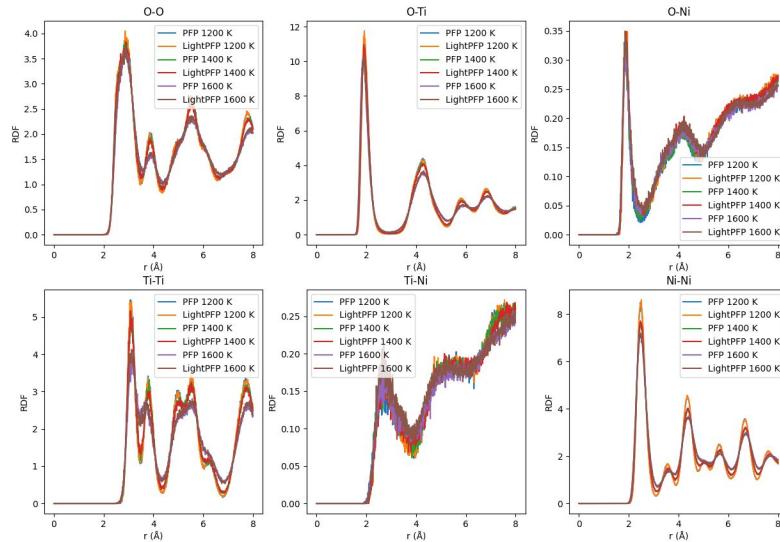
RDF: Small model; Ni (100) / TiO₂ (001) interface (Ti / O terminations)



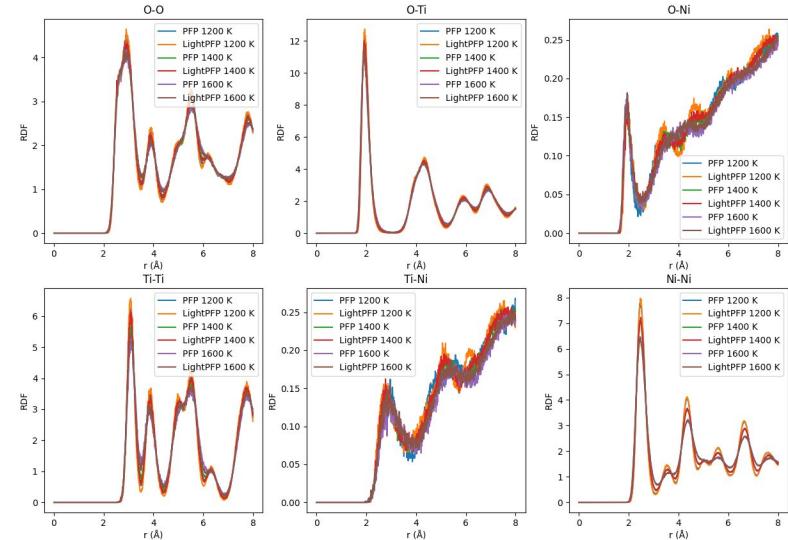
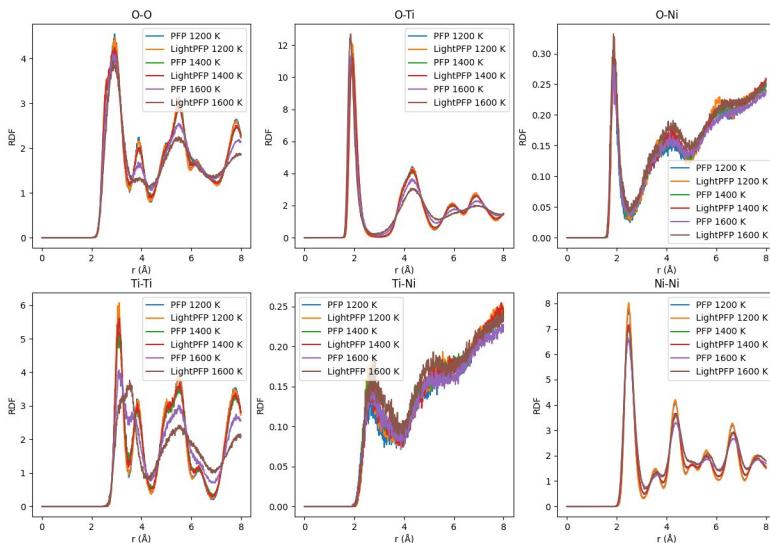
RDF: Large model; Ni (111) / TiO₂ (101) interface (Ti / O terminations)



RDF: Large model; Ni (110) / TiO₂ (001) interface (Ti / O terminations)



RDF: Large model; Ni (100) / TiO₂ (001) interface (Ti / O terminations)



Evaluation: MSD

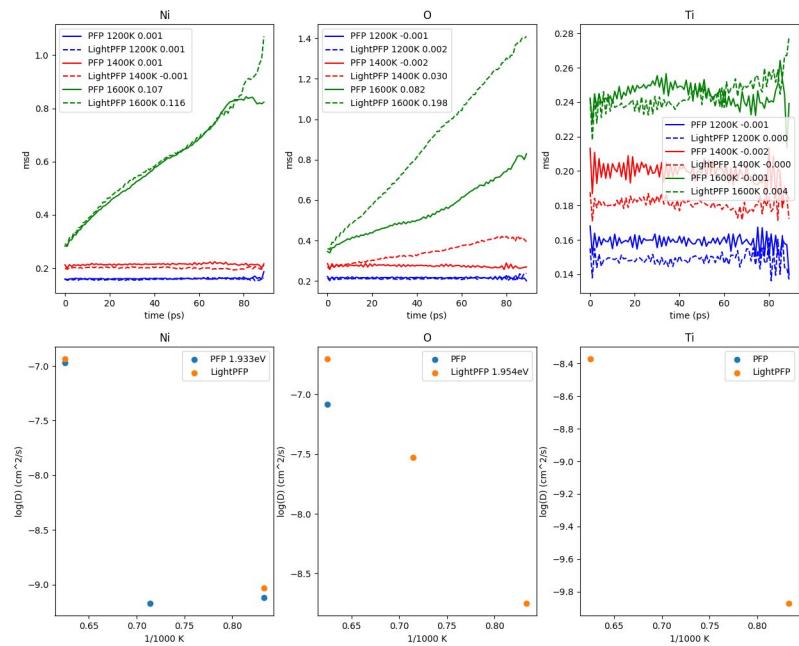
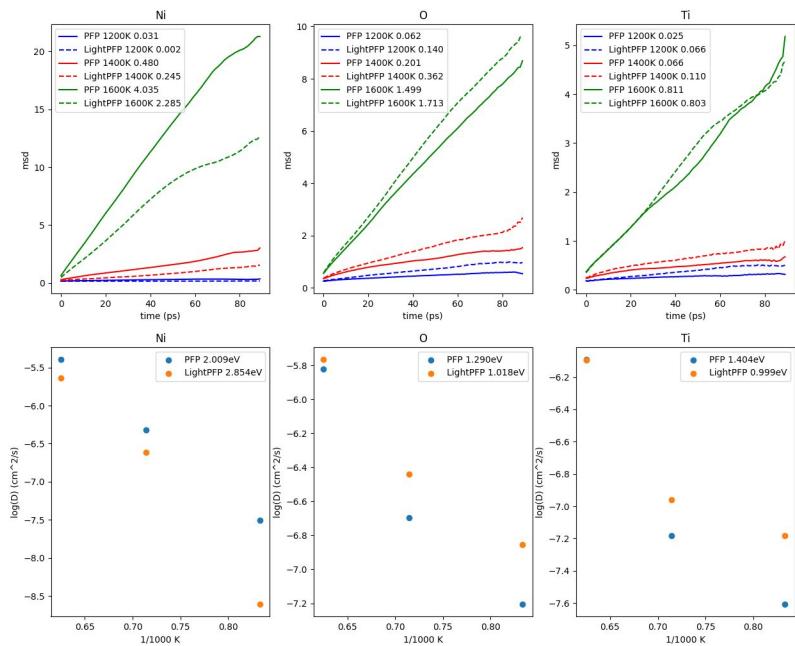
Diffusion coefficient

	Temperature	Ni Diffusion coefficient ($10^{-6} \text{ cm}^2/\text{s}$)			O Diffusion coefficient ($10^{-6} \text{ cm}^2/\text{s}$)			Ti Diffusion coefficient ($10^{-6} \text{ cm}^2/\text{s}$)		
		PFP	LightPFP small	LightPFP Large	PFP	LightPFP small	LightPFP Large	PFP	LightPFP small	LightPFP Large
Ni (111) / TiO ₂ (101) interface (Ti terminations)	1200K	0.031	0.002	0.012	0.062	0.14	0.03	0.025	0.066	0.02
	1400K	0.48	0.245	0.05	0.201	0.362	0.22	0.066	0.11	0.074
	1600K	4.035	2.285	4.198	1.499	1.713	1.584	0.811	0.803	0.72
Ni (111) / TiO ₂ (101) interface (O terminations)	1200K	0.001	0.001	-0.001	-0.001	0.002	0.002	-0.001	0	0.002
	1400K	0.001	-0.001	0.003	-0.002	0.03	0.001	-0.002	0	0.001
	1600K	0.107	0.116	-0.001	0.082	0.198	0.021	-0.001	0.004	0.002
Ni (110) / TiO ₂ (001) interface (Ti terminations)	1200K	0.176	0.177	0.115	0.335	0.416	0.236	0.014	0.124	0.029
	1400K	0.506	0.684	1.016	0.559	1.023	0.963	0.128	0.203	0.35
	1600K	3.061	2.549	2.608	2.716	3.35	2.307	1.443	1.354	0.983
Ni (110) / TiO ₂ (001) interface (O terminations)	1200K	0.006	0.006	0.003	0.007	0.052	0.021	0.013	0.006	0.012
	1400K	0.105	0.105	0.112	0.023	0.15	0.041	0.008	0.008	0.003
	1600K	0.878	1.211	1.348	0.397	0.645	0.353	0.019	0.112	0.006
Ni (100) / TiO ₂ (001) interface (Ti terminations)	1200K	0.201	0.148	0.172	0.204	0.351	0.239	0.036	0.111	0.073
	1400K	0.712	0.63	0.797	0.758	1.088	1.126	0.205	0.21	0.179
	1600K	3.091	3.143	3.728	2.807	3.723	5.499	1.375	1.752	3.184
Ni (100) / TiO ₂ (001) interface (O terminations)	1200K	0.075	0.035	0.123	0.007	0.001	0.001	0.004	-0.002	0
	1400K	0.41	0.245	0.33	0.093	0.11	0.033	0	0.017	-0.001
	1600K	2.121	1.903	1.551	0.576	1.111	0.402	0.009	0.139	0.004

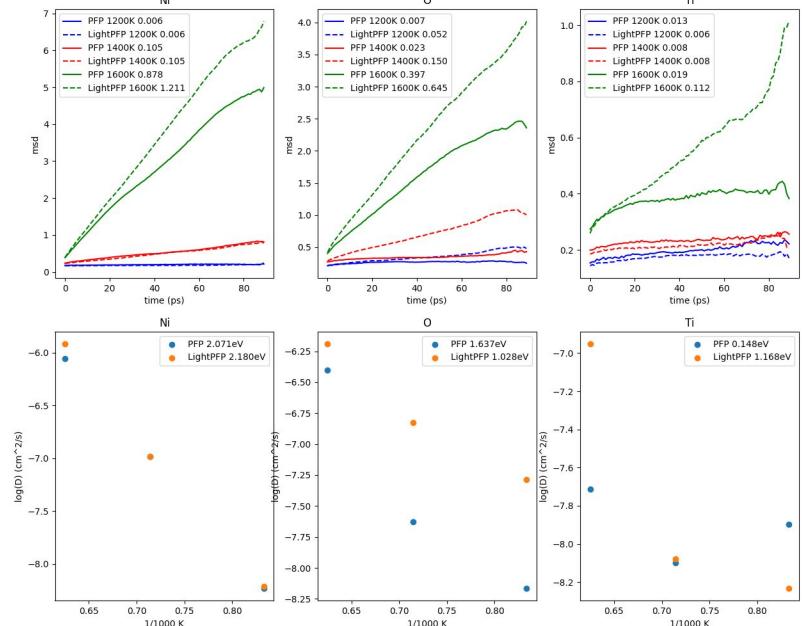
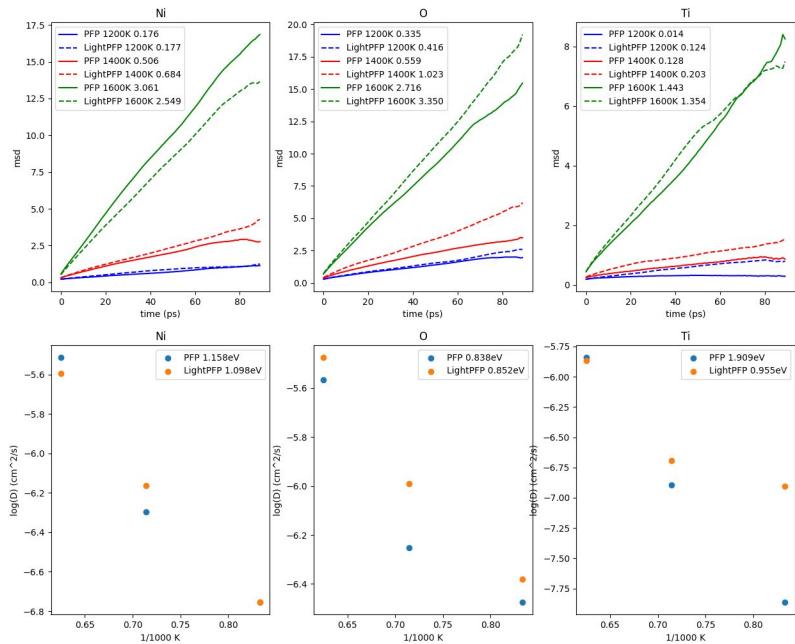
Diffusion activation energy

	Elements	Active energy (eV)			Active energy error (eV)	
		PFP	LightPFP small	LightPFP Large	LightPFP small	LightPFP Large
Ni (111) / TiO ₂ (101) interface (Ti terminations)	Ni	2.009	2.854	2.351	0.845	0.342
	O	1.29	1.018	1.625	0.272	0.335
	Ti	1.404	0.999	1.446	0.405	0.042
Ni (111) / TiO ₂ (101) interface (O terminations)	Ni	-	-	-		
	O	-	-	-		
	Ti	-	-	-		
Ni (110) / TiO ₂ (001) interface (Ti terminations)	Ni	1.158	1.098	1.305	0.06	0.147
	O	0.838	0.852	0.946	0.014	0.108
	Ti	1.909	0.955	1.47	0.954	0.439
Ni (110) / TiO ₂ (001) interface (O terminations)	Ni	2.071	2.18	2.543	0.109	0.472
	O	1.637	1.026	1.127	0.611	0.51
	Ti	-	-	-		
Ni (100) / TiO ₂ (001) interface (Ti terminations)	Ni	1.119	1.253	1.263	0.134	0.144
	O	1.078	0.968	1.288	0.11	0.21
	Ti	1.49	1.103	1.511	0.387	0.021
Ni (100) / TiO ₂ (001) interface (O terminations)	Ni	1.372	1.636	1.032	0.264	0.34
	O	-	-	-	-	-
	Ti	-	-	-	-	-
Average		1.448	25	1.329	1.492	0.347
						0.259

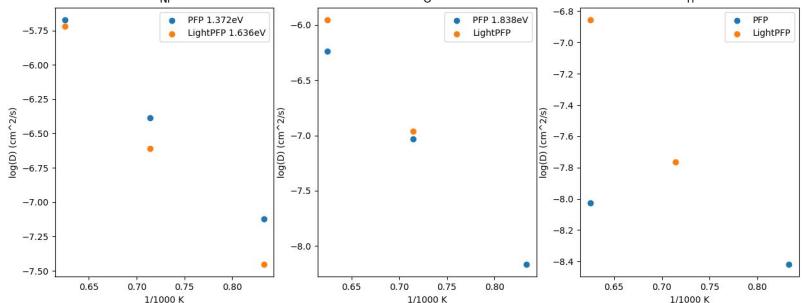
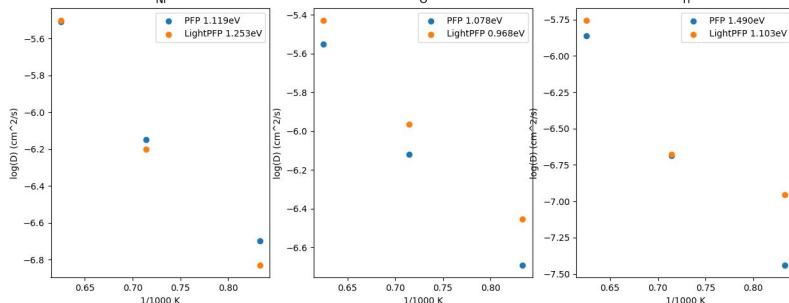
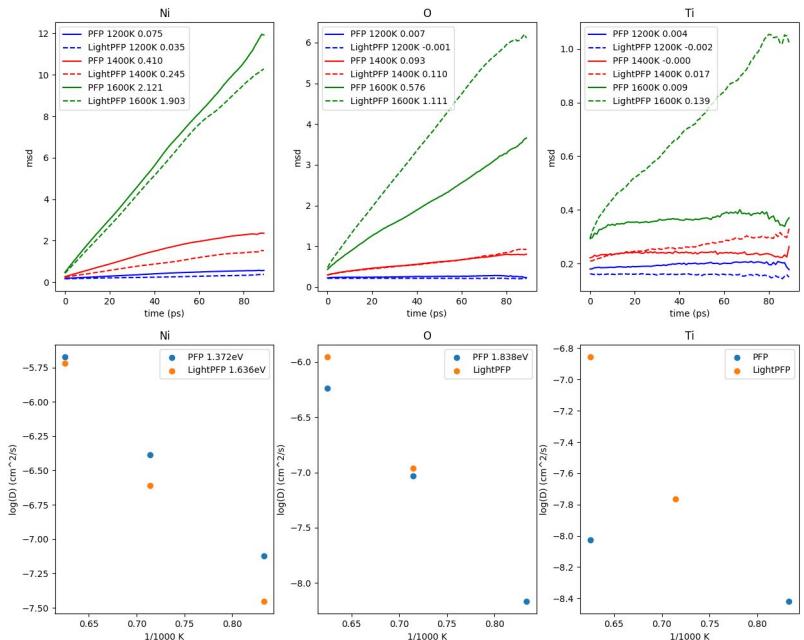
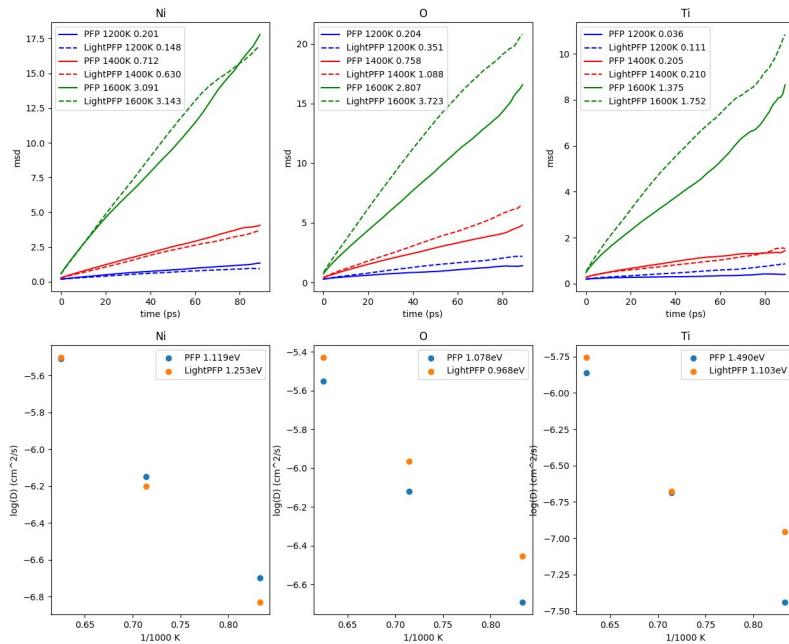
MSD: Small model; Ni (111) / TiO₂ (101) interface (Ti / O terminations)



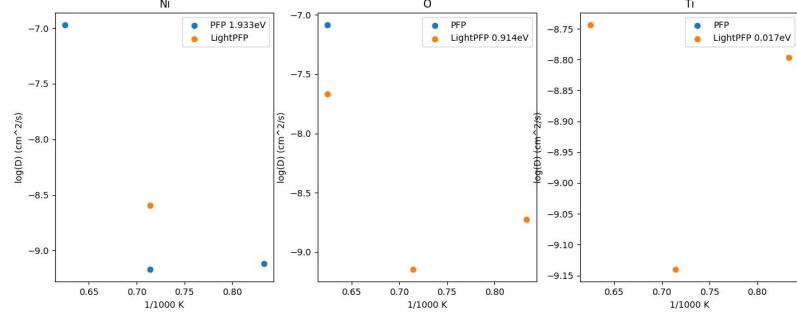
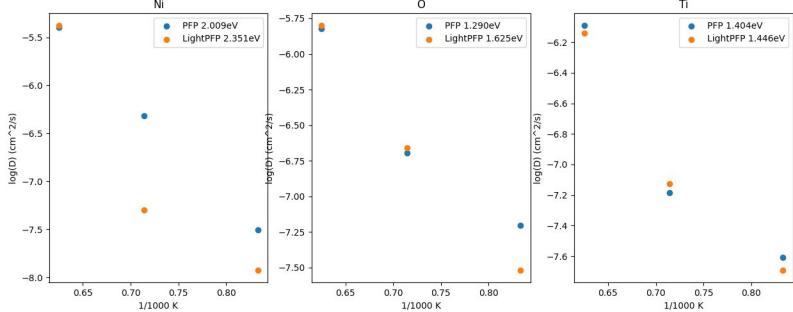
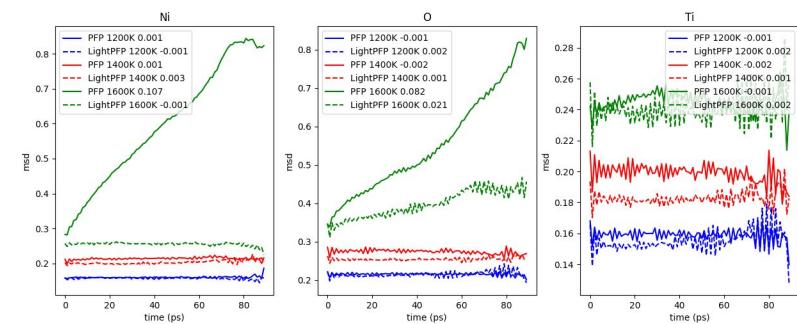
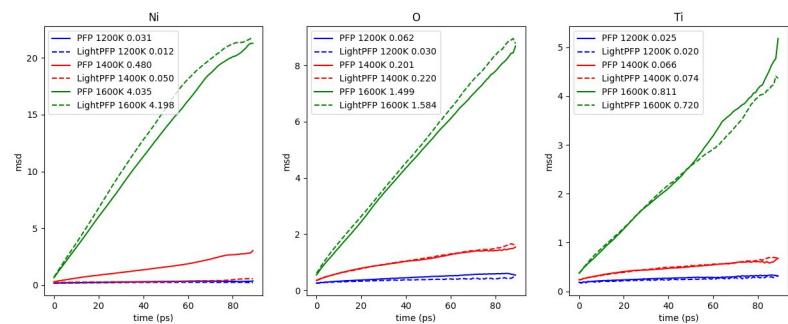
MSD: Small model; Ni (110) / TiO₂ (001) interface (Ti / O terminations)



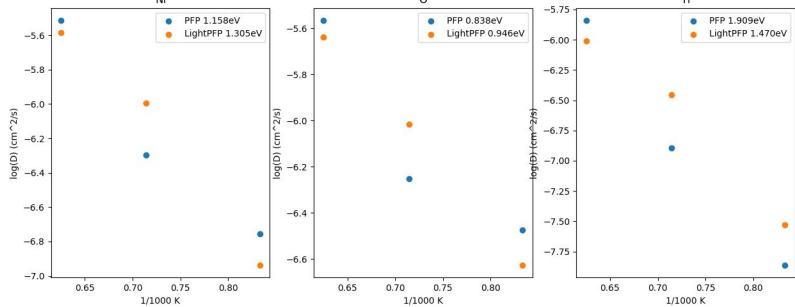
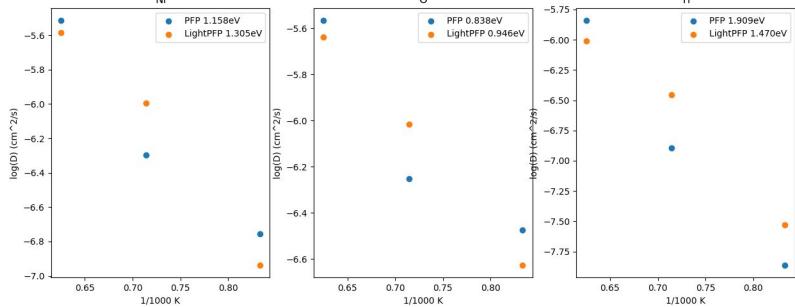
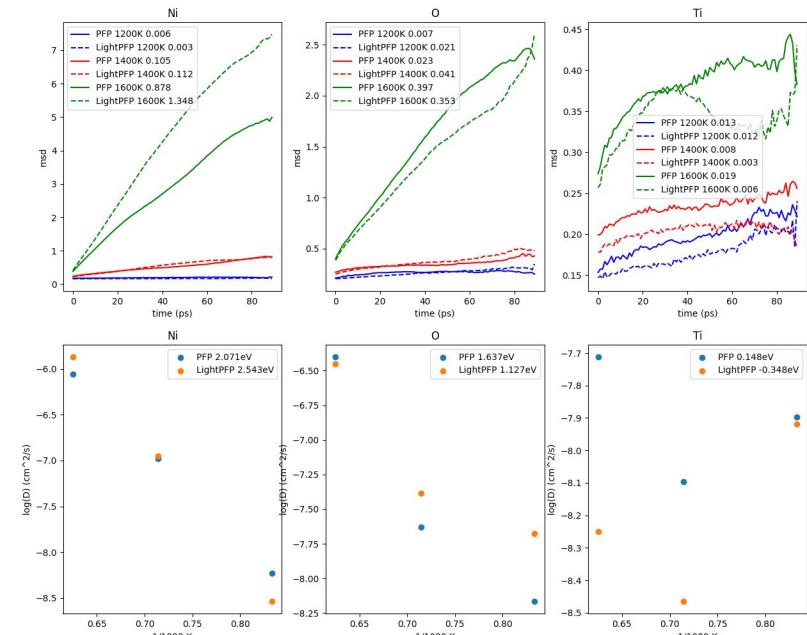
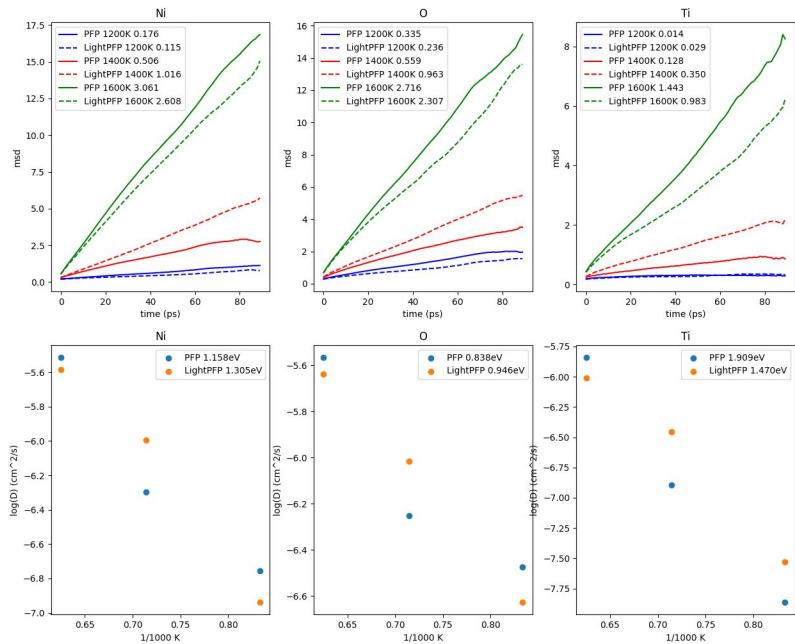
MSD: Small model; Ni (100) / TiO₂ (001) interface (Ti / O terminations)



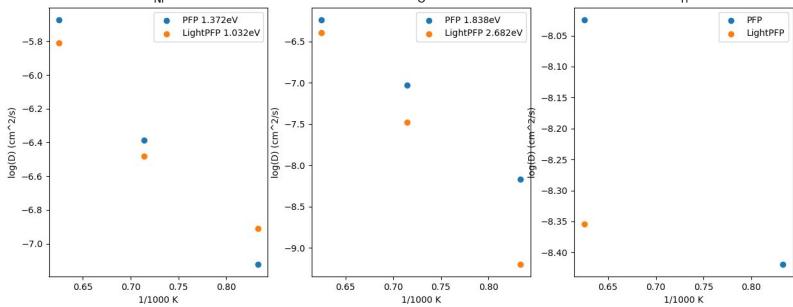
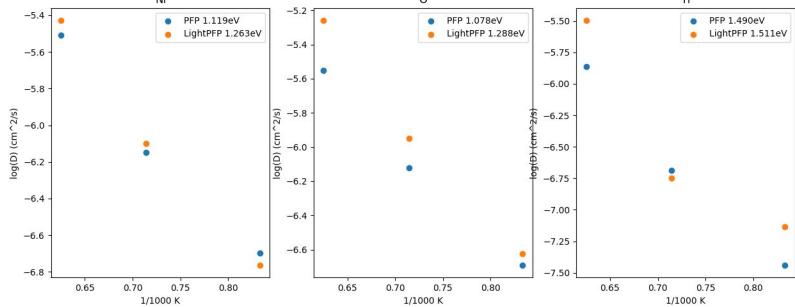
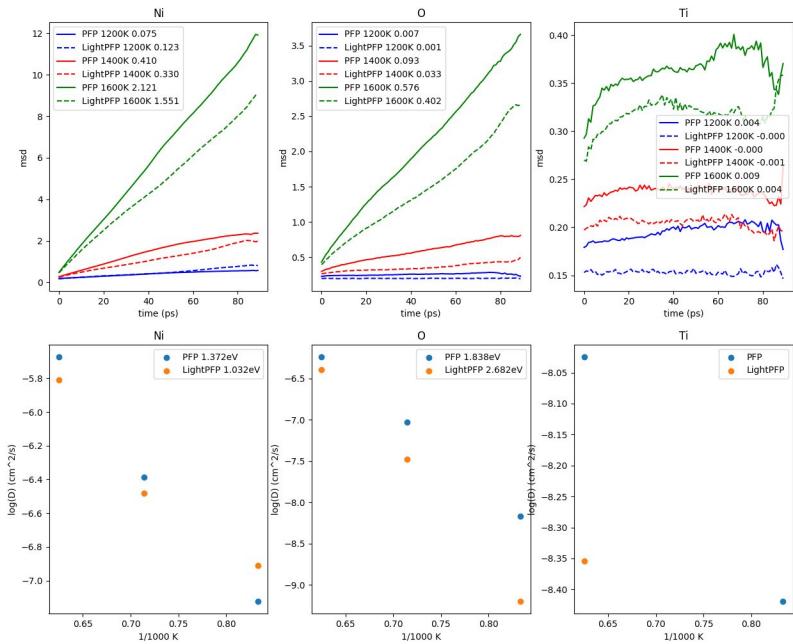
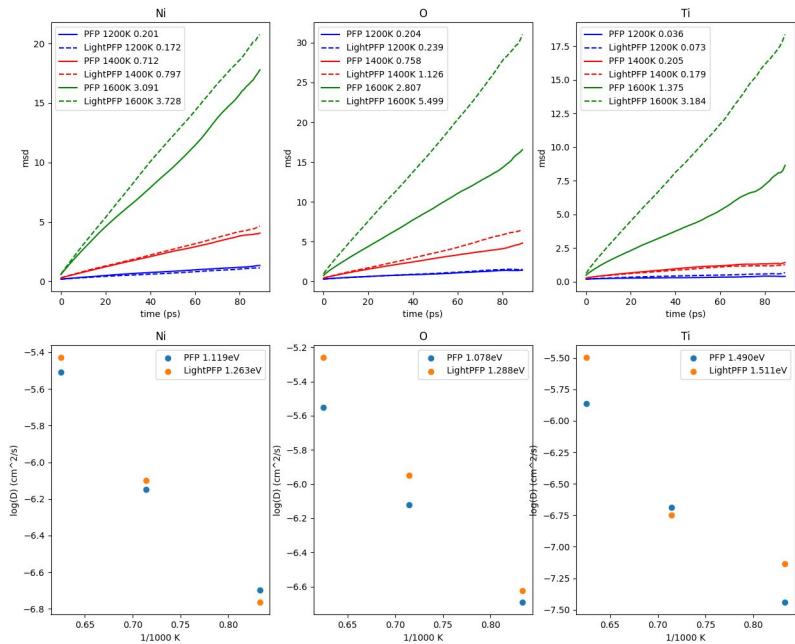
MSD: Large model; Ni (111) / TiO₂ (101) interface (Ti / O terminations)



MSD: Large model; Ni (110) / TiO₂ (001) interface (Ti / O terminations)

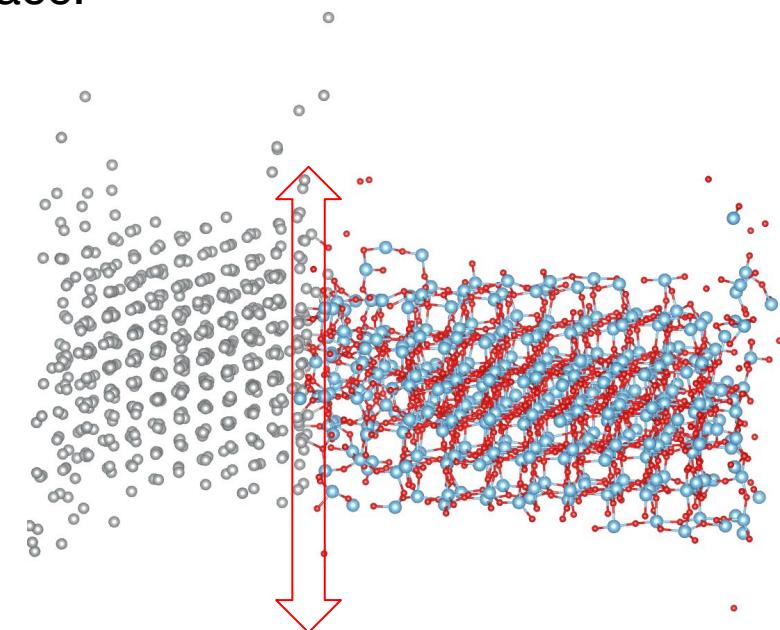
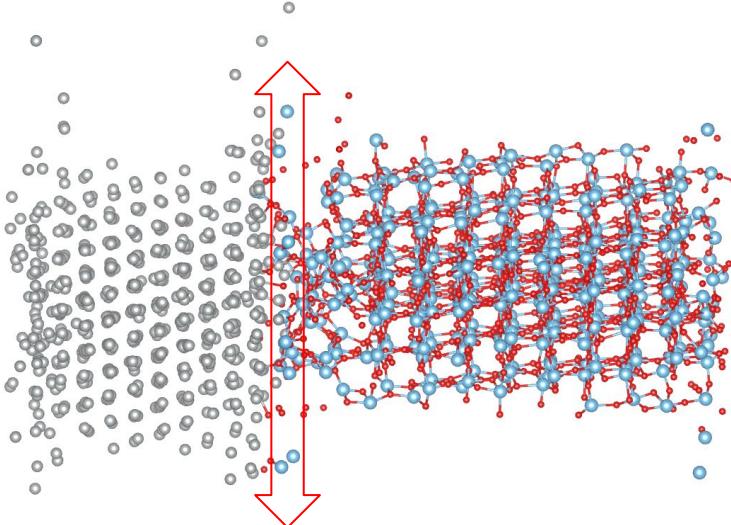


MSD: Large model; Ni (100) / TiO₂ (001) interface (Ti / O terminations)



Diffusion directions

- Diffusion:
 - Atomic diffusion occurs at interface.



Final Ni (111) / TiO₂ (101) interface structures (Ti termination) after 100 ps MD simulation at 1600 K

Evaluation: Interface energy

Interface energy

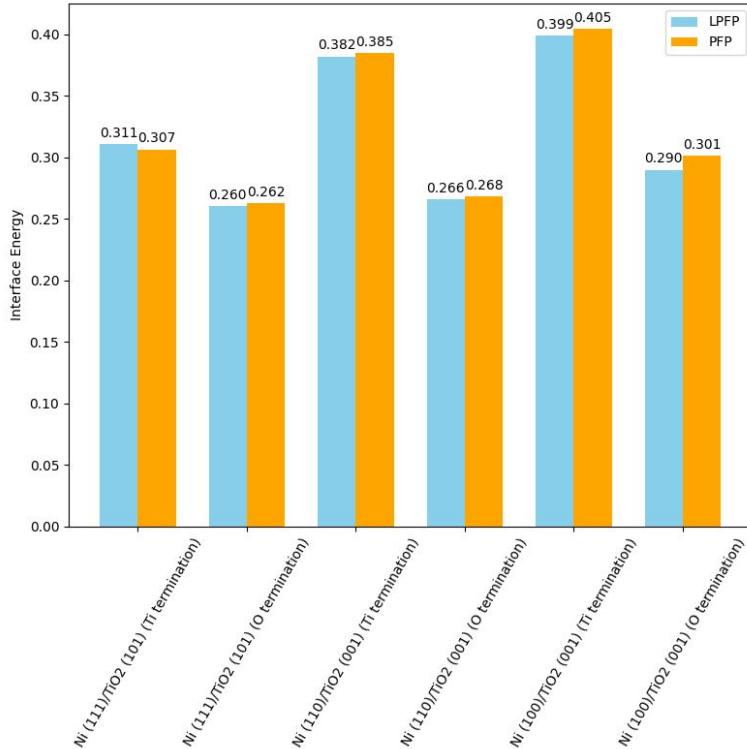
- Final frame of 1200K MD trajectory
- Structure optimization
- Calculate interface energy
 - $E_{\text{interface}} = E_{\text{Ni}_\text{TiO}_2} - E_{\text{Ni}} - E_{\text{TiO}_2}$

Interface energy

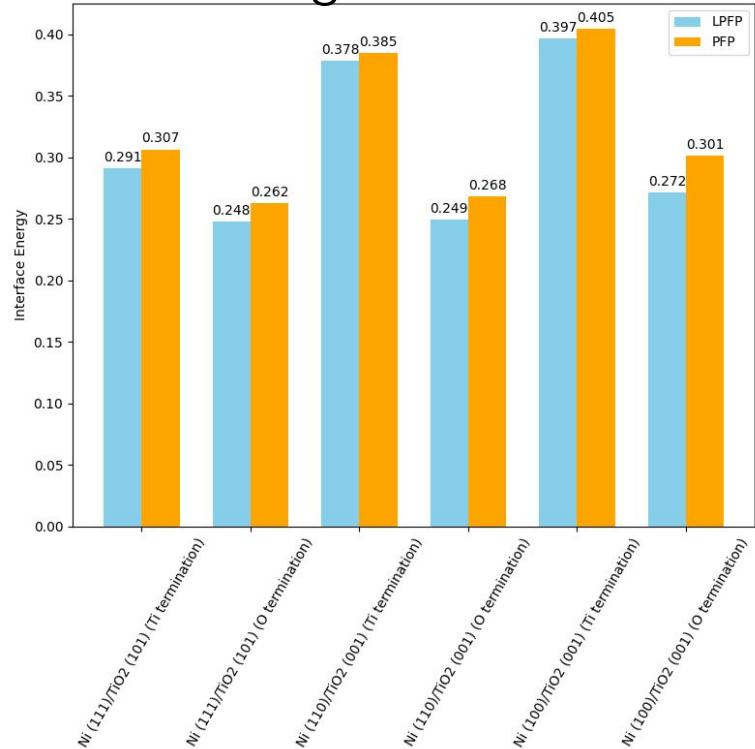
	Interface energy (eV)			Interface energy error (eV)	
	PFP	LightPFP small	LightPFP Large	LightPFP small	LightPFP Large
Ni (111) / TiO ₂ (101) interface (Ti terminations)	0.307	0.311	0.291	0.004	0.016
Ni (111) / TiO ₂ (101) interface (O terminations)	0.262	0.26	0.248	0.002	0.014
Ni (110) / TiO ₂ (001) interface (Ti terminations)	0.385	0.382	0.378	0.003	0.007
Ni (110) / TiO ₂ (001) interface (O terminations)	0.268	0.266	0.249	0.002	0.019
Ni (100) / TiO ₂ (001) interface (Ti terminations)	0.405	0.399	0.397	0.006	0.008
Ni (100) / TiO ₂ (001) interface (O terminations)	0.301	0.29	0.272	0.011	0.029
Average	0.3213	0.3180	0.3058	0.0047	0.0155

Interface energy

Small model



Large model



Thank you