

Pseudopotential	Formation Energy (eV)	Bulk Energy (Ry)	Vacancy Energy (Ry)	Avg Bulk Moment (μ <sub>B</sub> )	Avg Vac Moment (μ <sub>B</sub> )	Max Displacement (Å)	Mean Displacement (Å)
PAW	2.330	-17780.548607	-17451.107906	2.272	2.307	0.0769	0.0212
USPP	2.319	-13736.160714	-13481.616911	2.281	2.317	0.0781	0.0215