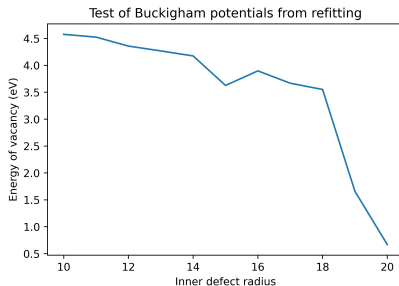
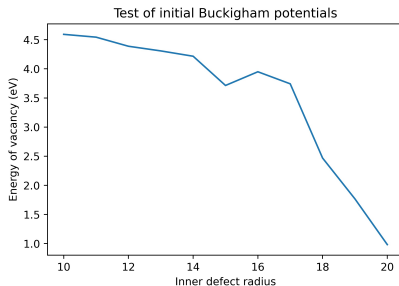


# Post-Christmas Update

Ben Goldmann

January 11, 2021

# Initial vs Refitted



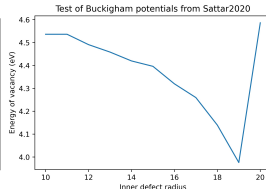
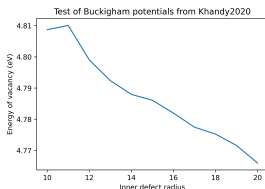
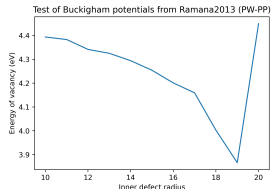
## Buckingham potentials

Na-O	1226.84	0.307	0	1225.11	0.307	0
Na-Cl	2314.70	0.290	0	2292.53	0.290	0

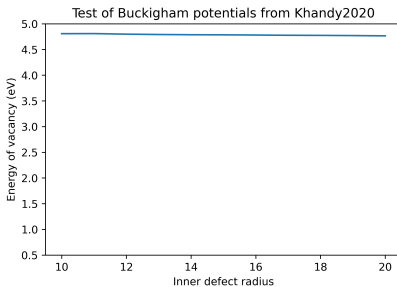
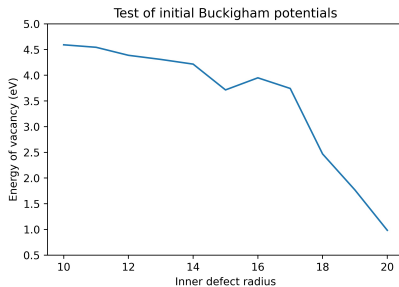
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# Data used and potentials calculated

Paper	Model	Bulk, GPa	Shear, GPa	Na-O Buckingham	Na-Cl Buckingham	Variation
Original	N/A	N/A	N/A	1226.84 0.307 0	2314.70 0.290 0	N/A
Ramana2013	FP-LAPW GGA	32.5	21.9	322.01 0.388 0	1727.87 0.297 0	3.55
Ramana2013	PW-PP GGA	34.2	22.9	369.22 0.376 0	1775.12 0.300 0	0.58
Deng2016	PAW GGA	36.4	24.6	1042.96 0.310 0	1591.38 0.288 0	20.35
Khandy2020	FP-LAPW GGA	33.45	26.87	588.38 0.338 0	1170.41 0.315 0	0.04
Sattar2020	FP-LAPW GGA	32.53	25.42	477.56 0.354 0	1270.12 0.309 0	0.61

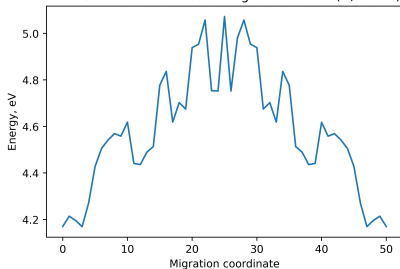


# Comparison of Initial and Khandy potentials

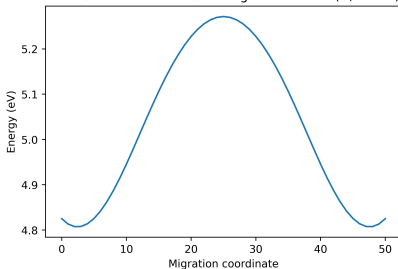


# Comparison of Initial and Khandy potentials

Na vacancy migration using initial potentials  
with defect centre fixed at migration centre (w/ shells)

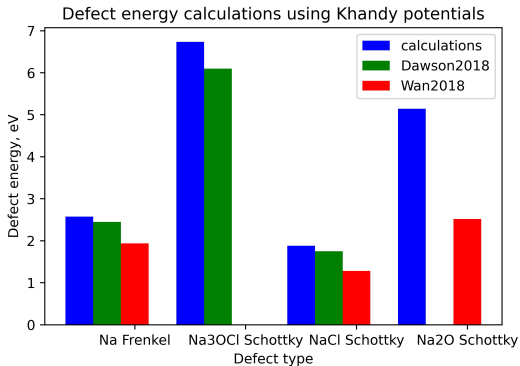


Na vacancy migration using Khandy potentials  
with defect centre fixed at migration centre (w/ shells)



# Calculations using potentials derived from Khandy2020

Parameter	Calc.	Comp. GGA	Comp. LDA	Comp. GULP	Experimental
lattice parameter, Å	4.41	4.54 <sup>1</sup> , 4.538 <sup>2</sup> , 4.53 <sup>3</sup> , 4.543 <sup>4</sup> , 4.514 <sup>4</sup> , 4.541 <sup>5</sup>	4.382 <sup>2</sup> , 4.381 <sup>4</sup> , 4.31 <sup>6</sup>	4.501 <sup>7</sup>	4.504 <sup>8</sup> , 4.496 <sup>9</sup> , 4.500 <sup>10</sup> , 4.4908 <sup>11</sup>
Na Frenkel, eV	2.58	1.94 <sup>1</sup> , 2.45 <sup>7</sup>			
NaCl Schottky, eV	1.88	1.28 <sup>1</sup> , 1.75 <sup>7</sup>			
Na <sub>2</sub> O Schottky, eV	5.14	2.52 <sup>1</sup>			
Na <sub>3</sub> OCl Schottky, eV	6.74	6.10 <sup>7</sup>			
Na vacancy migration, eV	0.46	0.61 <sup>1</sup> , 0.428 <sup>11</sup> , 0.29 <sup>8</sup> , 0.29 <sup>7</sup>			0.63 <sup>11</sup> , 1.04 <sup>8</sup>



# Review of results

- ▶ Concern over slightly off lattice parameter
- ▶ Discussion with Ben and Lucy
- ▶ They suggested that while the results may look good, they might not be accurate
- ▶ They proposed trying to fit the potentials using Lucy's code
- ▶ This involves thermally distorting the initial structure via AIMD, taking snapshots,, doing single-point calculations on the snapshots and fitting the potentials to them



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