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## Supplementary Information

### Electronic Structure, Ion Diffusion and Cation Doping in the Na<sub>4</sub>VO(PO<sub>4</sub>)<sub>2</sub> Compound as a Cathode Material for Na-ion Batteries

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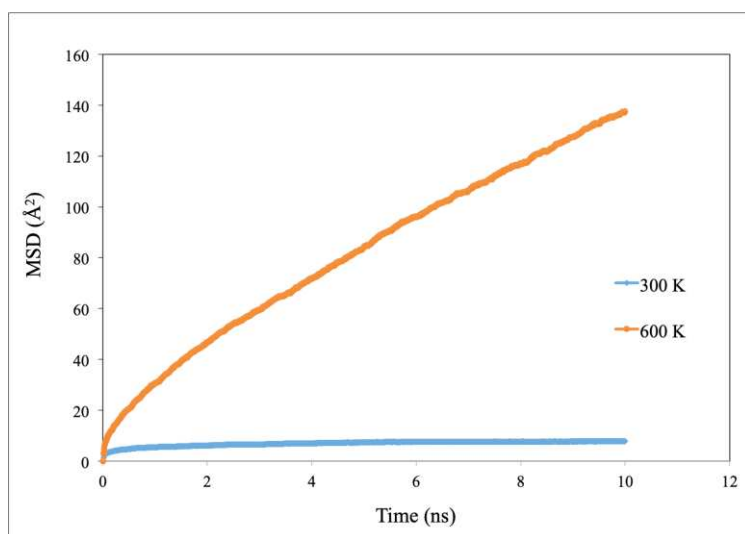
**Table SII.** Pedone interatomic potential parameters of NaVOPO<sub>4</sub> polymorphs.<sup>1</sup> The V-O parameters were optimized using the GULP software.<sup>2</sup>

<b>Buckingham: <math>Ae^{-r/\rho} - Cr^{-6}</math></b>	<b>A (eV)</b>	<b><math>\rho</math> (Å)</b>	<b>C (eV Å<sup>6</sup>)</b>	<b>Cut-off (Å)</b>
Na <sup>0.6</sup> -O <sup>-1.2</sup>	2010.33	0.261901	28.1687	$r_{\min} = 0.0/r_{\max} = 15.0$
P <sup>3</sup> -O <sup>-1.2</sup>	28357	0.178335	68.0998	$r_{\min} = 0.0/r_{\max} = 15.0$
V <sup>3</sup> -O <sup>-1.2</sup>	2306.19	0.228157	0	$r_{\min} = 0.0/r_{\max} = 15.0$
V <sup>2.4</sup> -O <sup>-1.2</sup>	2306.19	0.228157	0	$r_{\min} = 0.0/r_{\max} = 15.0$
O <sup>-1.2</sup> -O <sup>-1.2</sup>	2067.72	0.342846	214.2	$r_{\min} = 0.0/r_{\max} = 15.0$

**Table SI2.** Computed and experimental bond lengths of  $\beta$ -Na<sub>4</sub>VO(PO<sub>4</sub>)<sub>2</sub> compound (in Å).

		$\beta$ -Na <sub>4</sub> VO(PO <sub>4</sub> ) <sub>2</sub>	
	Comp.	Exp. <sup>a</sup>	
V-O	1.749	1.845	
	1.940	1.868	
	1.966	1.945	
	1.977	1.950	
	1.989	1.967	
	2.043	1.992	
P-O	1.527	1.518	
	1.542	1.519	
	1.561	1.529	
	1.564	1.615	
Na(1)-O	2.297	2.260	
	2.324	2.336	
	2.394	2.431	
	2.432	2.452	
	2.433	2.478	
	2.459	2.507	
Na(2)-O	2.243	2.223	
	2.247	2.234	
	2.312	2.285	
	2.329	2.414	
	2.712	2.657	
	2.816	2.853	
Na(3)-O	2.271	2.309	
	2.332	2.323	
	2.372	2.369	
	2.410	2.492	
Na(4)-O	2.325	2.301	
	2.460	2.489	
	2.470	2.536	
	2.517	2.600	
	2.617	2.623	
	2.624	2.698	
	2.823	2.756	

<sup>a</sup> Ref. <sup>3</sup>.



**Figure S11.** Mean square displacement (MSD) vs. time for the  $\text{Na}_4\text{VO}(\text{PO}_4)_2$  compound at 300 and 600 K.

### References

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