

Supplementary

Diffusion mechanism of Na ion – polaron complex in potential cathode materials NaVOPO₄ and VOPO₄ of rechargeable sodium-ion batteries

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Table S1: The on-site Coulomb U and the on-site exchange interaction J for GGA+U calculation

TYPES	U	J	Band gap (eV)
Liechtenstein approach ¹	4.2	0.7	2.179
	4.5	1.0	2.120
	5.6	0.7	2.120
	3.1	0.0	1.940
Dudarev approach ²	3.5	0.0	2.028
	3.8	0.0	2.066
	4.0	0.0	2.023

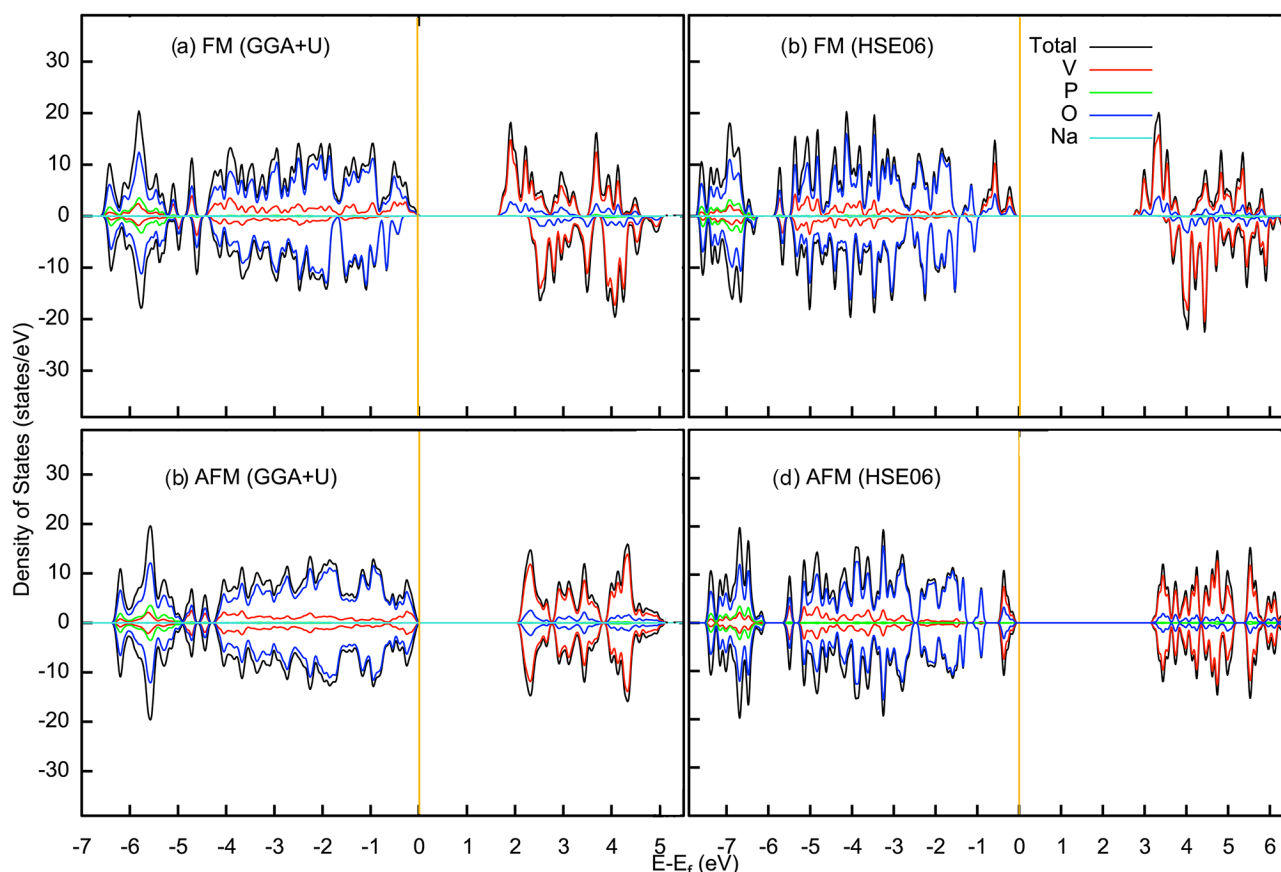


Figure S1: Density of state (DOS) of AFM and FM configurations of NaVOPO₄ obtained by GGA+U and HSE06. The negative (positive) value of DOS indicates the down (up) spin.

¹ A. I. Liechtenstein, V. I. Anisimov and J. Zaanen, Phys. Rev. B, 1995, 52, R5467.

² S. L. Dudarev, G. A. Botton, S. Y. Savrasov, C. J. Humphreys and A. P. Sutton, Phys. Rev. B, 1998, 57, 1505.

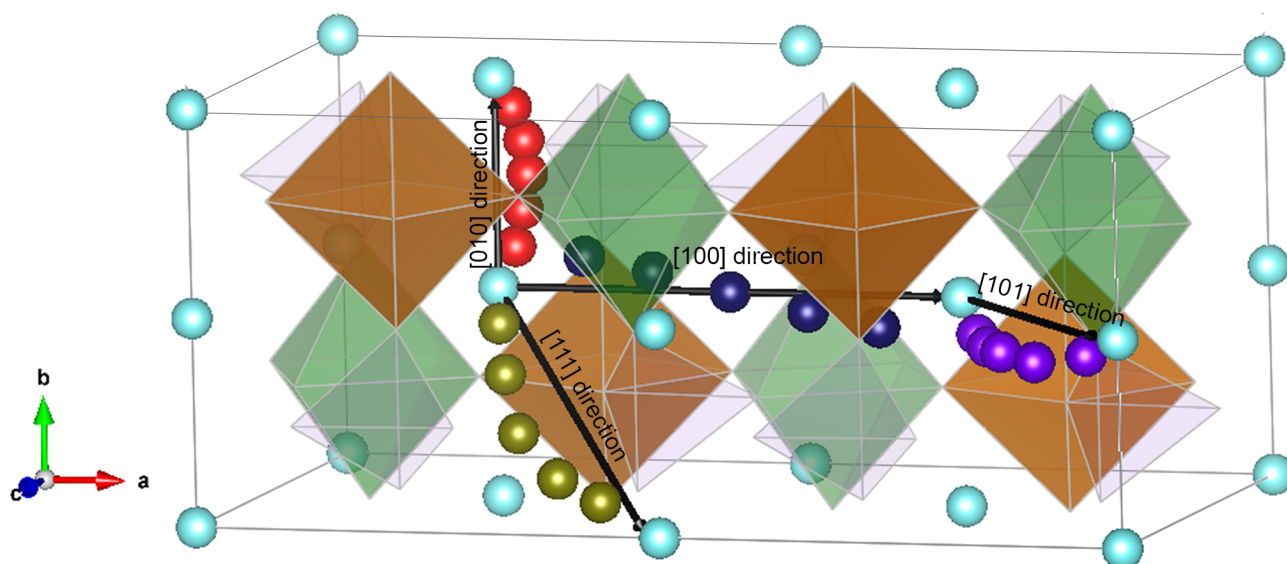


Figure S2: Diffusion directions in NaVOPO_4

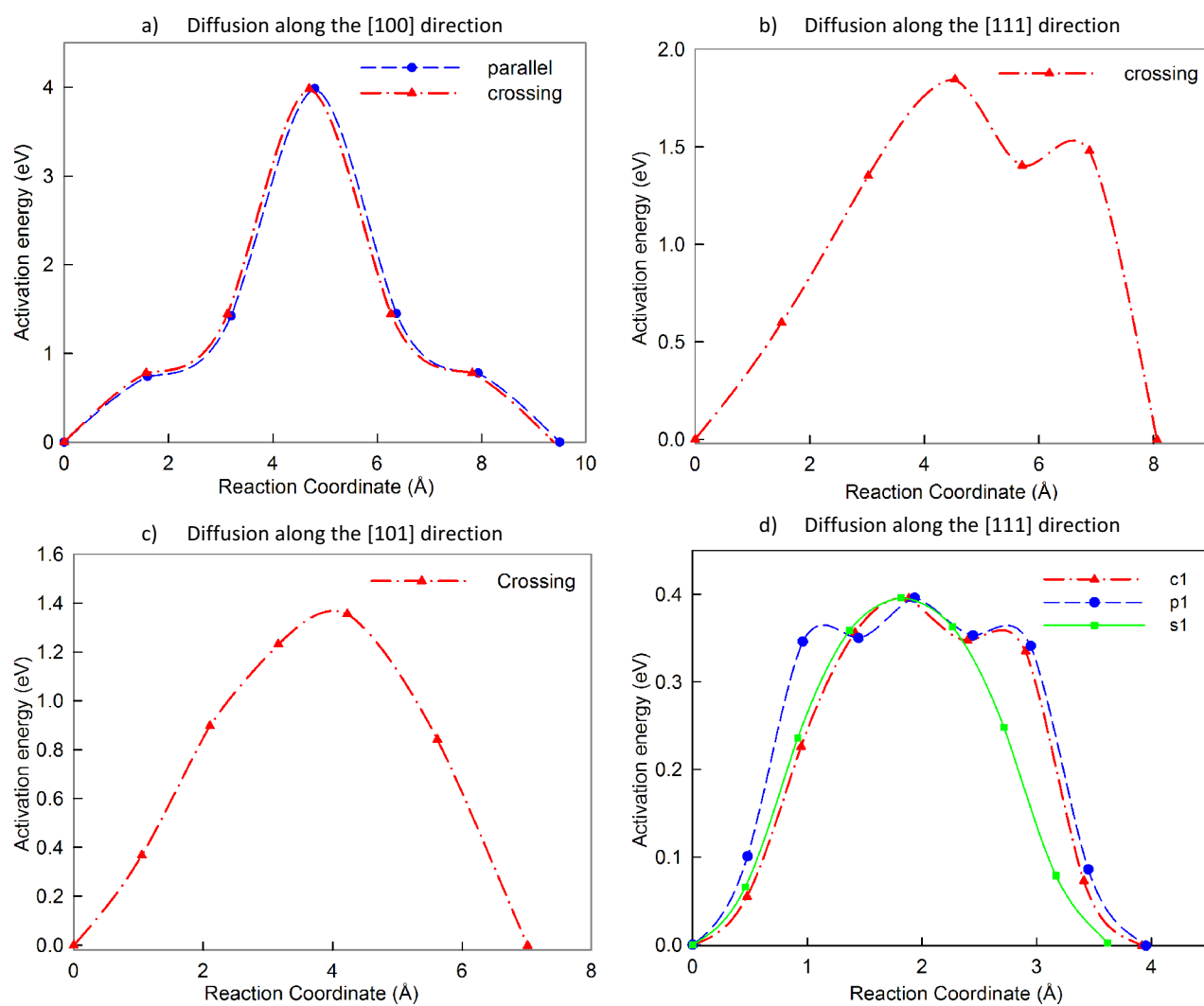


Figure S3: Activation energy profile of Na vacancy – positive polaron complex in NaVOPO_4 . The red, blue and green curves correspond to the crossing, parallel and single diffusion processes, respectively.

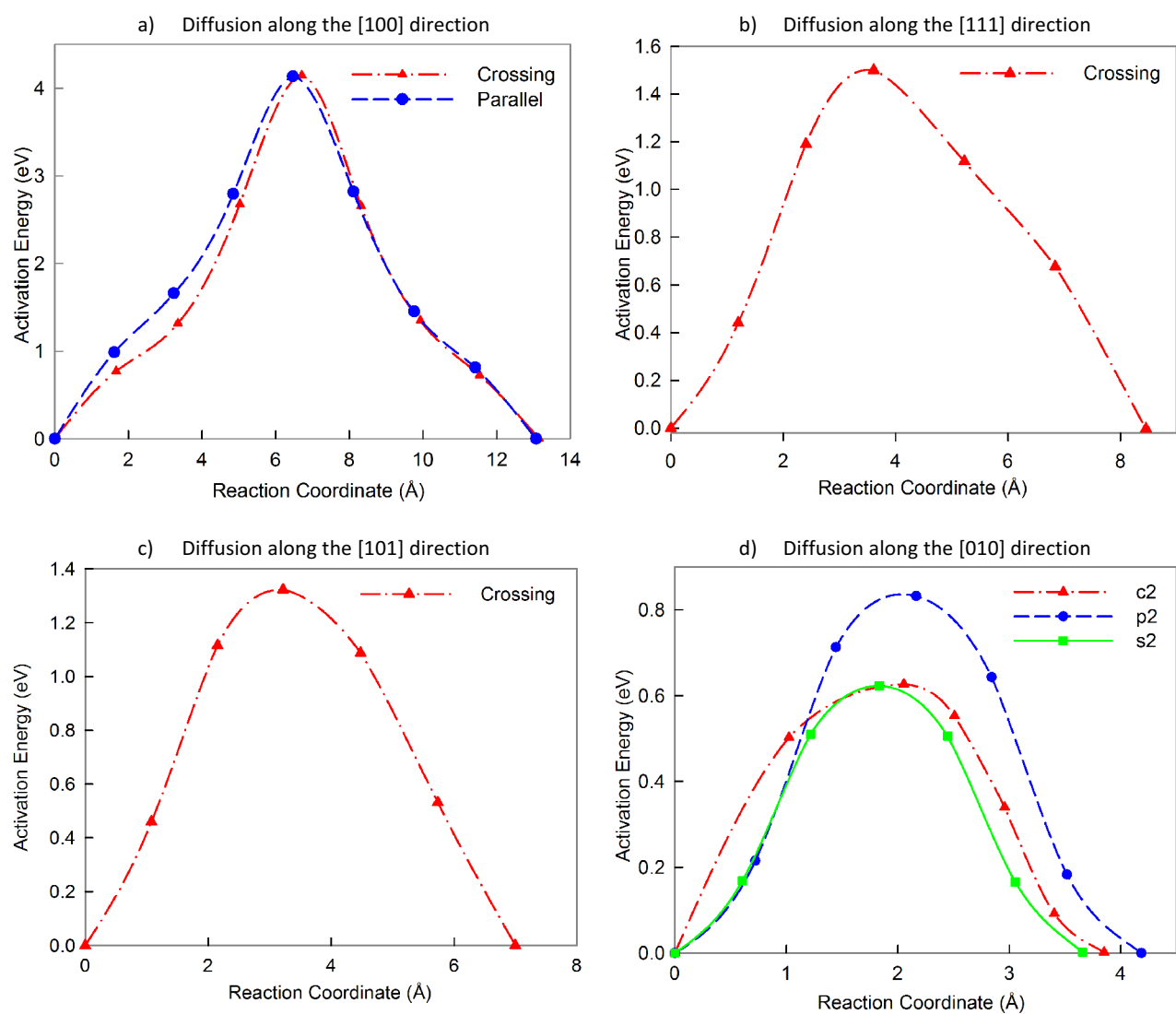


Figure S4: Activation energy profile of Na ion – negative polaron complex in VOPO_4 . Red, blue and green curves illustrate the crossing, parallel and single diffusion processes, respectively.