Supplementary Information for

Hydride Ion Intercalation and Conduction in the Electride Sr_3CrN_3

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Table S1. Coordinate(s) occupied by hydride ion(s) and the corresponding energy change.

Coordinate(s) occupied	$\triangle E$ (eV)	$\triangle E$ (eV/H)
(2/3, 1/3, 1/4)	0.24	0.24
(0, 0, 1/4)	-0.41	-0.41
(0, 0, 0)	-0.80	-0.80
(2/3, 1/3, 1/4), (1/3, 2/3, 3/4)	0.48	0.24
(0, 0, 1/4), (2/3, 1/3, 1/4)	-0.20	-0.10
(2/3, 1/3, 1/4), (0, 0, 0)	-0.68	-0.34
(0, 0, 1/4), (0, 0, 3/4)	-0.95	-0.48
(0, 0, 1/4), (0, 0, 0)	-1.90	-0.95
(0, 0, 0), (0, 0, 1/2)	-1.91	-0.96
(2/3, 1/3, 1/4), (1/3, 2/3, 3/4), (0, 0, 1/4)	-0.00	-0.00
(0, 0, 1/4), (2/3, 1/3, 1/4), (0, 0, 0)	-0.05	-0.02
(0, 0, 0), (0, 0, 1/2), (0, 0, 1/4)	-0.19	-0.06
(0, 0, 1/4), (2/3, 1/3, 1/4), (1/3, 2/3, 3/4)	-0.56	-0.19
(2/3, 1/3, 1/4), (1/3, 2/3, 3/4), (0, 0, 0)	-0.61	-0.20
(0, 0, 0), (0, 0, 1/2), (2/3, 1/3, 1/4)	-1.50	-0.50
(0, 0, 0), (0, 0, 1/4), (2/3, 1/3, 1/4)	-1.73	-0.58
(0, 0, 1/4), (0, 0, 3/4), (0, 0, 0), (0, 0, 1/2)	0.31	0.08
(0, 0, 0), (0, 0, 1/2), (2/3, 1/3, 1/4), (0, 0, 1/4)	-0.10	0.02
(0, 0, 1/4), (0, 0, 3/4), (2/3, 1/3, 1/4), (0, 0, 0)	-0.37	-0.09
(0, 0, 0) ,(0, 0, 1/2),(2/3, 1/3, 1/4), (1/3, 2/3, 3/4)	-1.15	-0.29
(2/3, 1/3, 1/4), (1/3, 2/3, 3/4), (0, 0, 1/4), (0, 0, 0)	-1.61	-0.40
(0, 0, 1/4), (0, 0, 3/4), (2/3, 1/3, 1/4), (0, 0, 0), (0, 0, 1/2)	0.39	0.08
(0, 0, 1/4), (0, 0, 3/4), (2/3, 1/3, 1/4), (0, 0, 0), (1/3, 2/3, 3/4)	0.11	0.02
(2/3, 1/3, 1/4), (1/3, 2/3, 3/4), (0, 0, 0) ,(0, 0, 1/2),(0, 0, 1/4)	-0.04	-0.01
(2/3, 1/3, 1/4), (1/3, 2/3, 3/4), (0, 0, 0), (0, 0, 1/2), (0, 0, 1/4), (0 ,0, 3/4)	0.77	0.13

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Table S2. HSE calculated band gap for sequential hydrogen saturation of the 2b Wyckoff site in a 1x1x2 supercell.

Number of hydrogens	Hydrogen position(s)	Band gap value (eV)
0	N/a	0.00
1	(0, 0, 0)	0.58
2 (adjacent configuration)	(0, 0, 0), (0, 0, 0.5)	0.77
2 (intermittent configuration)	(0, 0, 0), (0, 0, 0.25)	0.58
3	(0, 0, 0), (0, 0, 0.25), (0, 0, 0.5)	0.91
4	(0, 0, 0), (0, 0, 0.25), (0, 0, 0.5), (0, 0, 0.75)	2.99