Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Hydrogen Trapping Potential of Some Li – doped Star-like Clusters and Super-alkali Systems

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Table S1. NPA charges (Q_{NPA}, au) of the binding Li sites in $C_5Li_7^+$ and its $21H_2@C_5Li_7^+$ analogue at the M06/6-311+G(d,p) level.

Li Centers	Q_{NPA} in $C_5Li_7^+$	Q_{NPA} in $21H_2@C_5Li_7^+$
Li (6)	0.781	0.511
Li (7)	0.781	0.501
Li (8)	0.781	0.515
Li (9)	0.781	0.506
Li (10)	0.781	0.502
Li (11)	0.714	0.463
Li (12)	0.714	0.474

Table S2. NPA charges (Q_{NPA}, au) of the Li sites in $Si_5Li_7^+$ and its $3H_2@Si_5Li_7^+$ (eq and ax) analogues at the M06/6-311+G(d,p) level.

Li Centers	Q_{NPA} in $Si_5Li_7^+$	Q_{NPA} in $3H_2@Si_5Li_7^+$ (eq)	Q_{NPA} in $3H_2@Si_5Li_7^+$ (ax)
Li (1)	0.799	0.797	0.799
Li (2)	0.799	0.796	0.800
Li (3)	0.799	0.449	0.798
Li (4)	0.799	0.796	0.801
Li (5)	0.799	0.797	0.799
Li (6)	0.524	0.524	0.184
Li (7)	0.524	0.526	0.527

Li (3) binding site for $3H_2@Si_5Li_7^+$ (eq)

Li (6) binding site for $3H_2@Si_5Li_7^+$ (ax)

Table S3. NPA charges (Q_{NPA}, au) of the Li sites in $Ge_5Li_7^+$ and its $nH_2@Ge_5Li_7^+$ (n = 3, 2 for eq and ax respectively) analogues at the M06/6-311+G(d,p) level.

Li Centers	Q_{NPA} in $Ge_5Li_7^+$	Q_{NPA} in $3H_2@Ge_5Li_7^+$ (eq)	Q_{NPA} in $2H_2@Ge_5Li_7^+$ (ax)
Li (2)	0.798	0.793	0.798
Li 6)	0.797	0.465	0.795
Li (4)	0.798	0.797	0.795
Li (10)	0.799	0.797	0.800
Li (5)	0.799	0.792	0.798
Li (11)	0.500	0.490	0.208
Li (12)	0.500	0.480	0.483

Li (6) binding site for $3H_2@Ge_5Li_7^+$ (eq)

Li (11) binding site for $2H_2@Ge_5Li_7^+$ (ax)

Table S4. NPA charges (Q_{NPA}, au) of the Li sites in $Ge_5Li_7^+$ and its $nH_2@Ge_5Li_7^+$ (n = 3, 2 for eq and ax respectively) analogues at the M06/6-311+G(d,p) level.

Li Centers	Q_{NPA} in Si_4Li_4	Q_{NPA} in $3H_2@Si_4Li_4$	Q_{NPA} in Ge_4Li_4	Q_{NPA} in $3H_2@Ge_4Li_4$
Li (1)	0.645	0.648	0.644	0.640
Li 2)	0.645	0.647	0.644	0.639
Li (3)	0.645	0.647	0.644	0.245
Li (4)	0.645	0.237	0.644	0.640

Li (4) binding site for $3H_2@Si_4Li_4$

Li (3) binding site for $3H_2@Ge_4Li_4$

Table S5. NPA charges (Q_{NPA}, au) of the Li sites in BLi_6^+ and its $18H_2@BLi_6^+$ analogue at the M052X/6-311+G(d) level.

Li Centers	Q_{NPA} in BLi_6^+	Q_{NPA} in $18H_2@BLi_6^+$
Li (1)	0.731	0.433
Li (2)	0.731	0.441
Li (3)	0.731	0.447
Li (4)	0.731	0.434
Li (5)	0.731	0.445
Li (6)	0.731	0.425

Table S6. NPA charges (Q_{NPA}, au) of the Li sites in $O_2Li_5^+$ and its $14H_2@O_2Li_5^+$ analogue at the M052X/6-311+G(d) level.

Li Centers	Q_{NPA} in $O_2Li_5^+$	Q_{NPA} in $14H_2@O_2Li_5^+$
Li (1)	0.849	0.719
Li (2)	0.849	0.717
Li (3)	0.849	0.716
Li (6)	0.948	0.718
Li (7)	0.948	0.719

Table S7. NPA charges (Q_{NPA}, au) of the Li sites in $N_2Li_7^+$ and its $18H_2@N_2Li_7^+$ analogue at the M052X/6-311+G(d) level.

Li Centers	Q_{NPA} in $N_2Li_7^+$	Q_{NPA} in $18H_2@N_2Li_7^+$
Li (1)	0.720	0.581
Li (2)	0.715	0.586
Li (3)	0.715	0.617
Li (4)	0.868	0.620
Li (5)	0.873	0.614
Li (8)	0.873	0.631
Li (9)	0.868	0.627

Table S8. NPA charges (Q_{NPA}, au) of the Li sites in $C_2Li_9^+$ and its $13H_2@C_2Li_9^+$ analogue at the M052X/6-311+G(d) level.

Li Centers	Q_{NPA} in $C_2Li_9^+$	Q_{NPA} in $13H_2@C_2Li_9^+$
Li (1)	0.552	0.501
Li (2)	0.552	0.482
Li (3)	0.552	0.487
Li (4)	0.656	0.485
Li (5)	0.647	0.375
Li (6)	0.656	0.495
Li (7)	0.646	0.377
Li (8)	0.552	0.515
Li (9)	-2.366	-1.930

Table S9. NPA charges (Q_{NPA}, au) of the Li sites in $B_2Li_{11}^+$ and its $18H_2@B_2Li_{11}^+$ analogue at the M052X/6-311+G(d) level.

Li Centers	Q_{NPA} in $B_2Li_{11}^+$	Q_{NPA} in $18H_2@B_2Li_{11}^+$
Li (1)	0.614	0.170
Li (2)	0.522	0.154
Li (3)	0.618	0.161
Li (4)	0.521	0.150
Li (7)	0.187	0.242
Li (8)	0.187	0.224
Li (9)	0.290	0.198
Li (10)	0.437	0.186
Li (11)	0.605	0.494
Li (12)	0.558	0.328
Li (13)	0.605	0.497

Table S10. NPA charges (Q_{NPA}, au) of the Li sites in $F_2Li_3^+$ and its $11H_2@F_2Li_3^+$ analogue at the M052X/6-311+G(d) level.

Li Centers	Q_{NPA} in $F_2Li_3^+$	Q_{NPA} in $11H_2@F_2Li_3^+$
Li (2)	0.970	0.748
Li (3)	0.925	0.858
Li (5)	0.970	0.749

Table S11. NPA charges (Q_{NPA}, au) of the Li sites in FLi_2^+ and its $8H_2@FLi_2^+$ analogue at the M052X/6-311+G(d) level.

Li Centers	Q_{NPA} in FLi_2^+	Q_{NPA} in $8H_2@FLi_2^+$
Li (1)	0.977	0.753
Li (2)	0.977	0.755

Table S12. NPA charges (Q_{NPA}, au) of the Li sites in OLi_3^+ and its $9H_2@OLi_3^+$ analogue at the M052X/6-311+G(d) level.

Li Centers	Q_{NPA} in OLi_3^+	Q_{NPA} in $9H_2@OLi_3^+$
Li (1)	0.938	0.751
Li (2)	0.938	0.749
Li (3)	0.938	0.750

Table S13. The variation of interaction energy per hydrogen molecule (ΔE, kcal/mol) with the variation of applied field strength (F, au) at the M052X/6-311+G(d) level.

Clusters	F	ΔE
$1H_2@BLi_6^+$	0.000	-2.46
	0.001 (-X)	-2.78
	0.002 (-X)	-3.24
	0.003 (-X)	-3.84
	0.004 (-X)	-4.61
	0.005 (-X)	-5.56
$1H_2@O_2Li_5^+$	0.000	-2.6
	0.001 (X)	-2.9
	0.002 (X)	-3.2
	0.003 (X)	-3.6
	0.004 X)	-4.0
	0.005 (X)	-4.5
	0.000	-1.9

$1H_2@N_2Li_7^+$	0.001 (Y)	-2.3
	0.002 (Y)	-2.7
	0.003 (Y)	-3.3
	0.004 (Y)	-4.0
	0.005 (Y)	-4.8
$1H_2@FLi_2^+$	0.000	-3.48
	0.001 (-X)	-3.89
	0.002 (-X)	-4.31
	0.003 (-X)	-4.74
	0.004 (-X)	-5.03
	0.005 (-X)	-5.66

(X) and (-X) mean the external electric field has been applied along X and –X direction respectively whereas (Y) means the external electric field has been applied along Y direction.