

Supplementary Information

Co-mixing Hydrogen and Methane May Double the Energy Capacity

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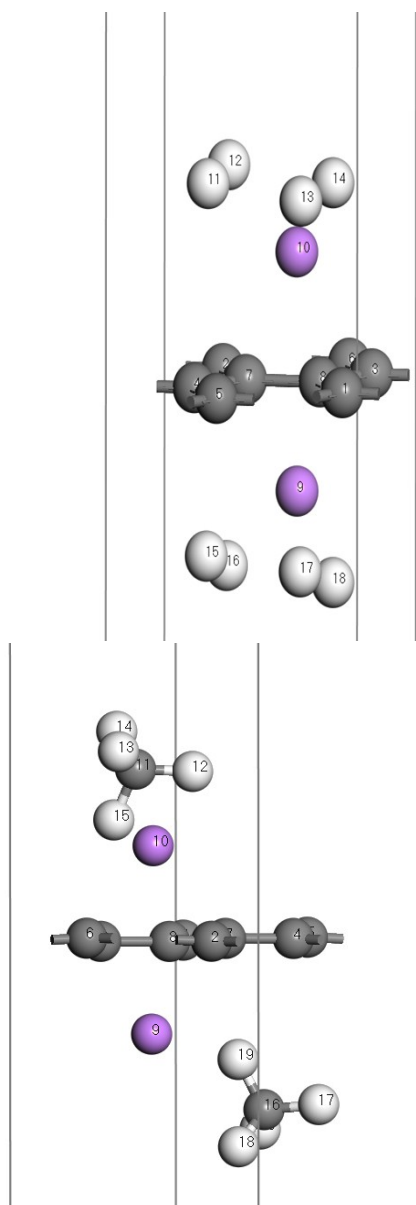
Figure S1 Hirshfeld charge analysis of various adsorption configurations in Fig. 3.

2 H₂ per Li

C	1 charge	-0.0217
C	2 charge	-0.0371
C	3 charge	-0.0410
C	4 charge	-0.0259
C	5 charge	-0.0410
C	6 charge	-0.0398
C	7 charge	-0.0375
C	8 charge	-0.0372
Li	9 charge	0.2027
Li	10 charge	0.2024
H	11 charge	-0.0119
H	12 charge	-0.0176
H	13 charge	-0.0123
H	14 charge	-0.0192
H	15 charge	-0.0124
H	16 charge	-0.0192
H	17 charge	-0.0122
H	18 charge	-0.0181

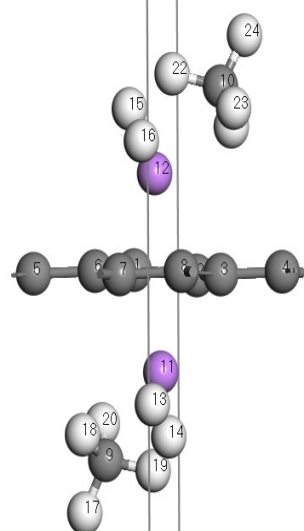
1CH₄ per Li

C	1 charge	-0.0393
C	2 charge	-0.0571
C	3 charge	-0.0605
C	4 charge	-0.0399
C	5 charge	-0.0550
C	6 charge	-0.0600
C	7 charge	-0.0578
C	8 charge	-0.0552
Li	9 charge	0.2459
Li	10 charge	0.2469
C	11 charge	-0.1523
H	12 charge	0.0259
H	13 charge	0.0246
H	14 charge	0.0330
H	15 charge	0.0346



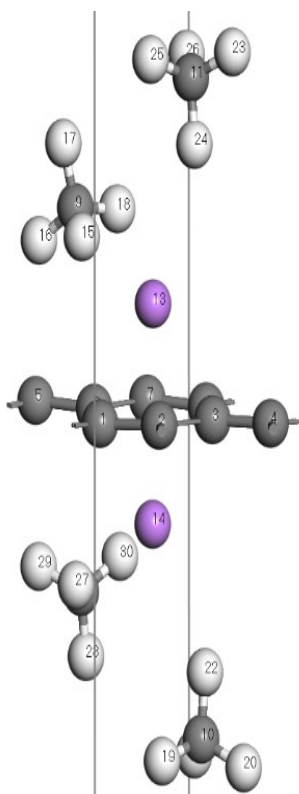
C	16	charge	-0.1538
H	17	charge	0.0263
H	18	charge	0.0337
H	19	charge	0.0341
H	20	charge	0.0268

1H₂+1CH₄ per Li



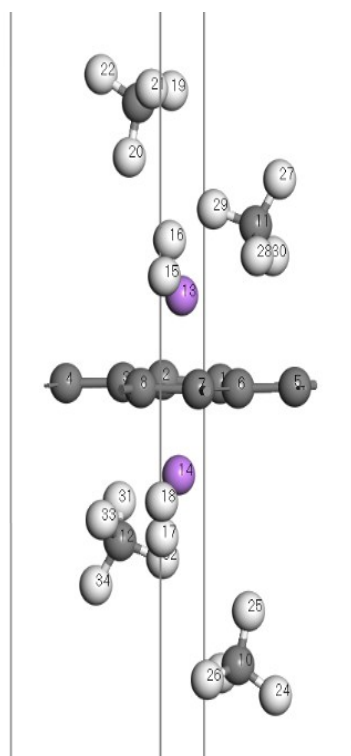
C	1	charge	-0.0559
C	2	charge	-0.0563
C	3	charge	-0.0556
C	4	charge	-0.0398
C	5	charge	-0.0399
C	6	charge	-0.0557
C	7	charge	-0.0510
C	8	charge	-0.0506
C	9	charge	-0.1434
C	10	charge	-0.1445
Li	11	charge	0.2079
Li	12	charge	0.2086
H	13	charge	0.0008
H	14	charge	-0.0131
H	15	charge	-0.0130
H	16	charge	0.0004
H	17	charge	0.0432
H	18	charge	0.0423
H	19	charge	0.0262
H	20	charge	0.0390
H	21	charge	0.0398
H	22	charge	0.0259
H	23	charge	0.0427
H	24	charge	0.0428

2CH₄ per Li



C	1	charge	-0.0567
C	2	charge	-0.0538
C	3	charge	-0.0533
C	4	charge	-0.0444
C	5	charge	-0.0370
C	6	charge	-0.0468
C	7	charge	-0.0520
C	8	charge	-0.0577
C	9	charge	-0.1400
C	10	charge	-0.1565
C	11	charge	-0.1586
C	12	charge	-0.1376
Li	13	charge	0.2532
Li	14	charge	0.2419
H	15	charge	0.0288
H	16	charge	0.0288
H	17	charge	0.0450
H	18	charge	0.0305
H	19	charge	0.0312
H	20	charge	0.0322
H	21	charge	0.0319
H	22	charge	0.0250

H	23	charge	0.0326
H	24	charge	0.0235
H	25	charge	0.0322
H	26	charge	0.0313
H	27	charge	0.0252
H	28	charge	0.0413
H	29	charge	0.0283
H	30	charge	0.0326



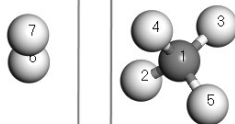
H	28	charge	0.0393
H	29	charge	0.0346
H	30	charge	0.0383
H	31	charge	0.0405
H	32	charge	0.0362
H	33	charge	0.0408
H	34	charge	0.0441

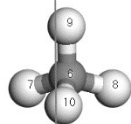
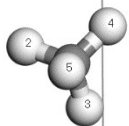
1H₂ + 2CH₄ per Li

C	1	charge	-0.0610
C	2	charge	-0.0573
C	3	charge	-0.0632
C	4	charge	-0.0359
C	5	charge	-0.0366
C	6	charge	-0.0633
C	7	charge	-0.0555
C	8	charge	-0.0593
C	9	charge	-0.1604
C	10	charge	-0.1612
C	11	charge	-0.1377
C	12	charge	-0.1388
Li	13	charge	0.2214
Li	14	charge	0.2245
H	15	charge	0.0069
H	16	charge	-0.0018
H	17	charge	-0.0025
H	18	charge	0.0072
H	19	charge	0.0335
H	20	charge	0.0297
H	21	charge	0.0328
H	22	charge	0.0339
H	23	charge	0.0327
H	24	charge	0.0337
H	25	charge	0.0296
H	26	charge	0.0319
H	27	charge	0.0435

1H₂ + 1CH₄

C	1	charge	-0.1284
H	2	charge	0.0361
H	3	charge	0.0365
H	4	charge	0.0362
H	5	charge	0.0370
H	6	charge	-0.0075
H	7	charge	-0.0084





2CH₄

C 1 charge
H 2 charge
H 3 charge
H 4 charge
H 5 charge
C 6 charge
H 7 charge
H 8 charge
H 9 charge
H 10 charge

-0.1291
0.0327
0.0318
0.0327
0.0315
-0.1277
0.0330
0.0333
0.0316
0.0328

2H₂

H 1 charge
H 2 charge
H 3 charge
H 4 charge



0.0003
0.0002
0.0003
0.0007