Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information

Revising the pathways of Li reaction with organic carbonates

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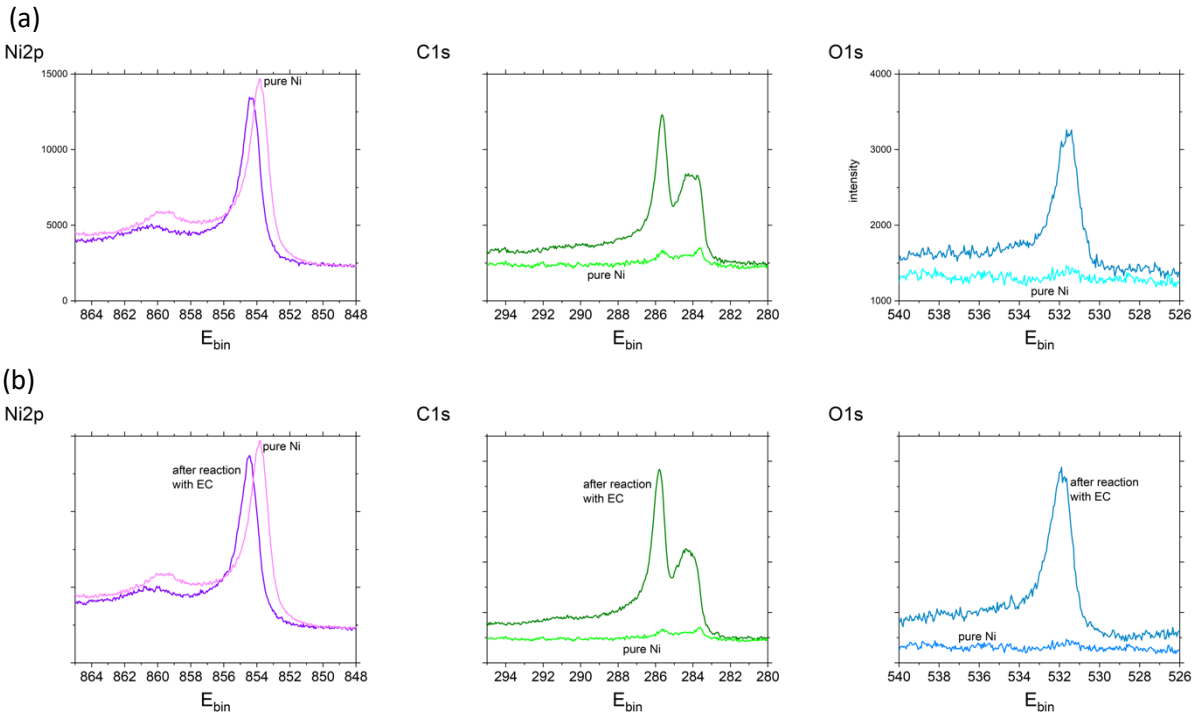

Figure S1. Spectra of clean Ni surface and surface of Ni after reaction with (a) PC (b) EC.

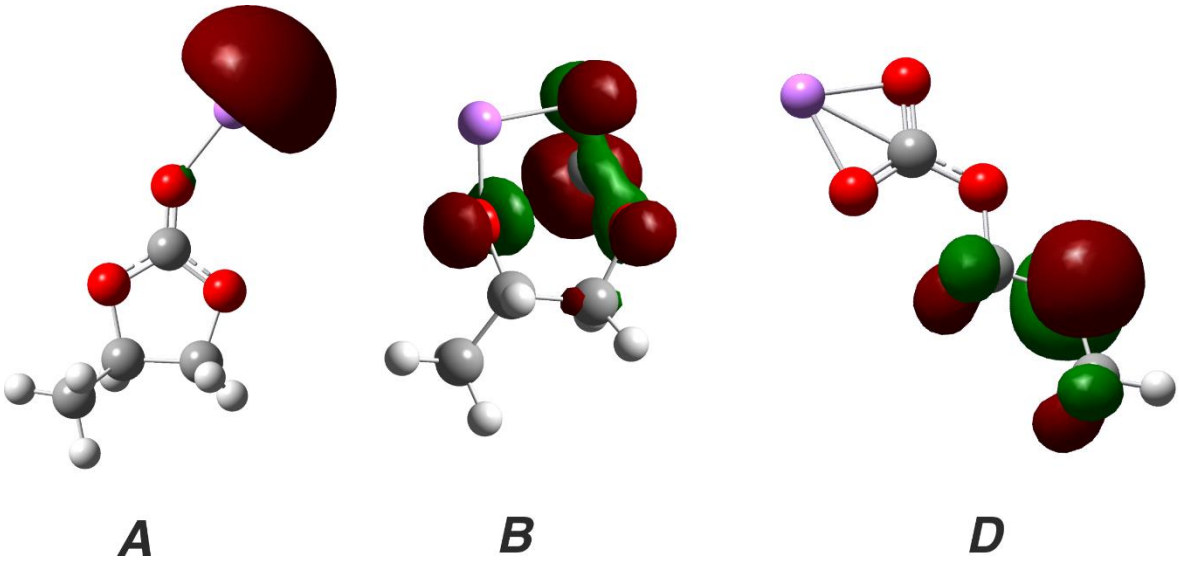

Figure S2. Isosurface plots of an unpaired electron charge density at a value=0.05 for A, B, D radicals.

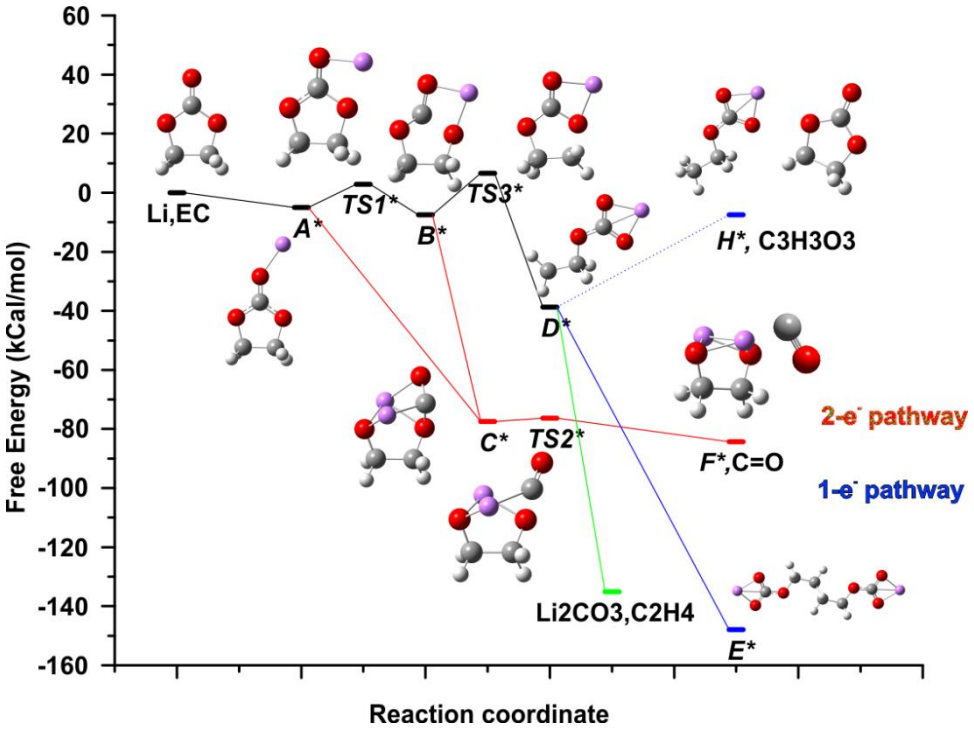

Figure S3. Energy diagram of the reaction between Li atoms and ethylene carbonate molecules.

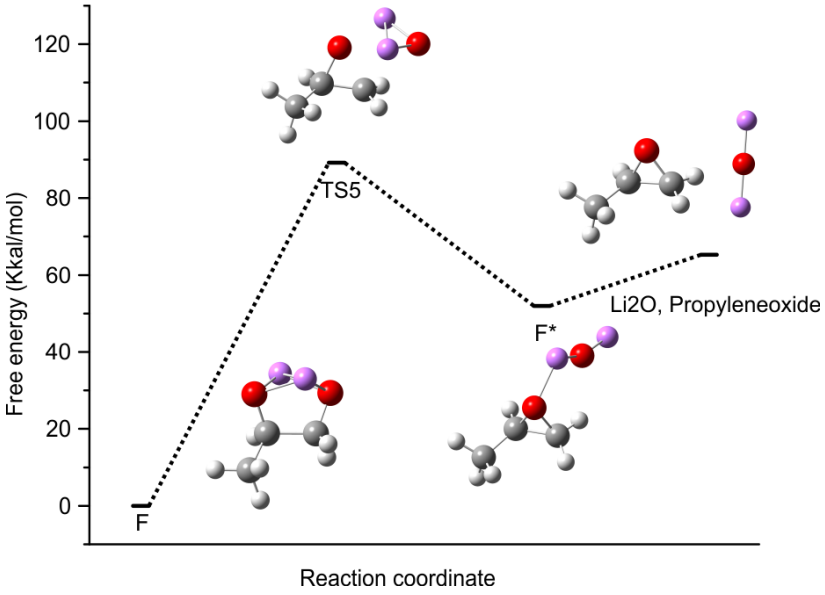

Figure S4. Energy diagram of the decomposition of DD into Li_2O

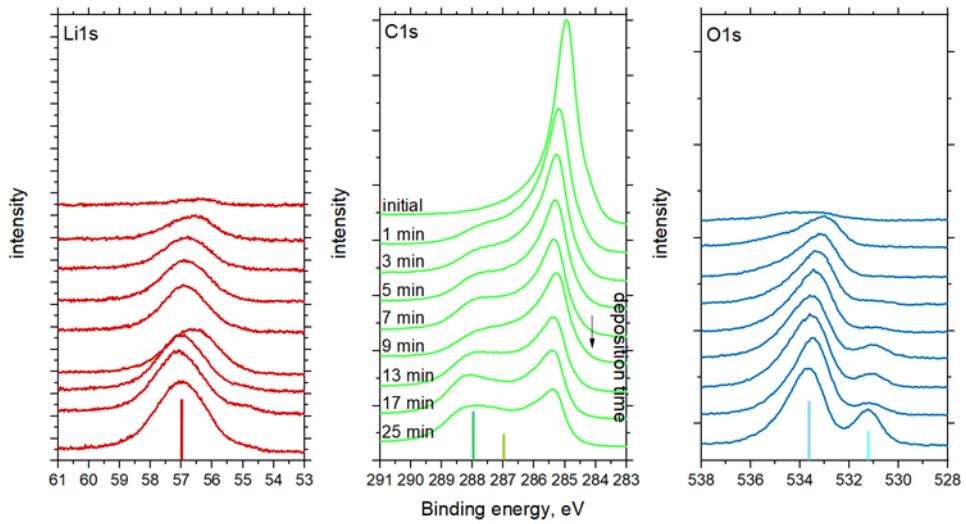

Figure S5. Spectra of lithium deposited on graphene in PC.

	Li		O		C			
	Li1	**Li2**	**O1**	**O2**	**C1**	**C2**	**C3**	**C4**
0	55.5	54.6	532.2	529.8			284.5	283.0
	20206	11472	782	3413			3006	2907
1	56.1	55.0	532.6	530.0	287.7	286.8	284.3	282.9
	22998	6444	5088	5186	8365	3715	3339	3592
2	56.2	55.2	532.4	529.9	287.6	286.6	284.5	283.1
	23265	8659	8803	7859	17187	6778	1410	4506
3	55.7	55.1	532.2	529.7	287.3	286.3	284.6	283.2
	25484	5453	15490	6617	18940	6622	334	3275
4	55.7	55.0	532.1	529.6	287.2	286.3	284.5	283.2
	26902	4423	15574	7393	26121	12043	379	3978
5	55.6	55.0	531.9	529.4	287.0	286.1	284.6	283.3
	25405	6947	17352	7971	25076	11809	569	5057

Table S1. Binding energies and absolute intensities of different components of spectra in figure 2

N	Li		O			C				
	Li1	**Li2**	**O3**	**O1**	**O2**	**C1**	**C2**	**C3**	**C4**	**C5**
0				530.9				285.3	283.9	283.3
				4647				16677	15758	2679
1	56.0		532.8	531.6		286.7	285.6	284.8	283.8	283.3
		12366	6979	8464		30150	7715	12879	6742	1957
2	55.7		532.6	531.8	529.4	287.0	285.9	284.7	284.0	283.3
		20210	8170	7819	3530	32664	11948	6226	3171	7258
3	56.0	55.3	532.1		529.6	287.4	286.4	284.7		283.4
	6117	21455	16896		6011	28726	15639		11848	4691
4	56.3	55.5	532.3		529.8	287.4	286.5	284.5		283.4
	19745	12105	16641		6181	32207	16063		11518	3811

Table S2. Binding energies and absolute intensities of different components of spectra in figure 3

N	Li		O			C				
	Li1	**Li2**	**O3**	**O1**	**O2**	**C1**	**C2**	**C3**	**C4**	**C5**
0				531.0				285.2	283.9	283.4
				5050				18538	8000	3566
2	56.1		532.2	531.3		286.4	285.6	285.0	283.9	283.4
		6177	5036	4958		9576	5446	30436	6260	949
4	56.1		532.7	531.5		286.6	285.9	284.9	283.8	283.3
		10167	5774	7743		17903	2687	24089	2473	2134
6	56.1		533.0	531.8	529.5	286.8	285.7	284.9	283.7	283.4
		17026	6168	11601	352	26697	4381	15743	2206	2208
9	56.3	55.4	532.5		529.9	287.5	286.6	285.8	283.6	283.4
	26435	10987	19753		7517	40049	3851	8508	1856	3067
10	56.4	55.4	532.6		530.0	287.6	286.4	285.8		283.5
	31539	8164	21236		8758	41063	3210		10112	4315

Table S3. Binding energies and absolute intensities of different components of spectra in figure 4