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

Supplementary Information for:

Enhanced field-emission properties of buckled α-borophene by Li decoration: A first-principles investigation

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Theoretical details for calculating field emission current:

The Penn-Plummer model was adopt to DFT calculations for the computation of the field-emission currents.[1] In DFT calculations, the supercell is generally discretized by introducing a fine grid. This grid divides the supercell face perpendicular to the emission direction into small surface elements. The emission current I_ι was calculated along individual grid lines parallel to the emission direction. The currents $I_\iota(\omega)$ can be expressed as[1-3]

$$I_\iota(\omega) = \frac{2e\hbar}{m_e} f(\omega) S_i \lambda_i^{-2}(\omega) D_i^2(\omega) g_i(\omega, x_{l,i}) \tag{1}$$

in which m_e is the electron effective mass, $f(\omega)$ is the Fermi-Dirac distribution, and S_i is the area of the surface element *i*. $\lambda_i(\omega)$ is a slowly varying function of the energy resulting from the asymptotic matching of the wave function of emitting state at the left turning point $x_{l,i}$ with WKB wave function inside the barrier. The left and right turning points, $x_{l,i}$ and $x_{r,i}$, along the grid line *i* are determined as the points where the energy of the emitting state becomes equal with the potential energy barrier $u_i(x)$, with *x* being the coordinate along the emission direction. $D_i^2(\omega)$ indicates the probability of electron tunneling through the nanostructure-vacuum barrier $u_i(x)$, and $g_i(\omega, x_{l,i})$ is the local density of states (LDOS) at the left turning point. $\lambda_i(\omega)$ is given by

$$\lambda_i(\omega) = (\pi/3)^{1/2} (c_i/3)^{-1/3} \left[\Gamma(2/3)\cos(\pi/6)\right]^{-1} \tag{2}$$

In eq. (2), c_i is obtained by fitting $(2m_e/\hbar^2)(u_i(x)-\omega)$ to $c_i^2(x - x_{l,i})$ at the left turning point. The tunneling probability $D_i^2(\omega)$ is given by

$$D_i^2(\omega) = \exp\left[-2\sqrt{\frac{2m_e}{\hbar}}\int_{x_{l,i}}^{x_{r.i}} \sqrt{u_i(x)-\omega dx}\right] \tag{3}$$

Actually, the emission current $I_\iota(\omega)$ was obtained based the necessary data (LDOS, $u_i(x)$, and $g_i(\omega, x_{l,i})$, which have been calculated by DMol[3].

REFERENCES

1. D. R. Penn and E. W. Plummer, *Phys. Rev. B*, 1974, **9**, 1216–1222.

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3. M. Khazaei, A. A. Farajian and Y. Kawazoe, *Phys. Rev. Lett.*, 2005, **95**, 177602.

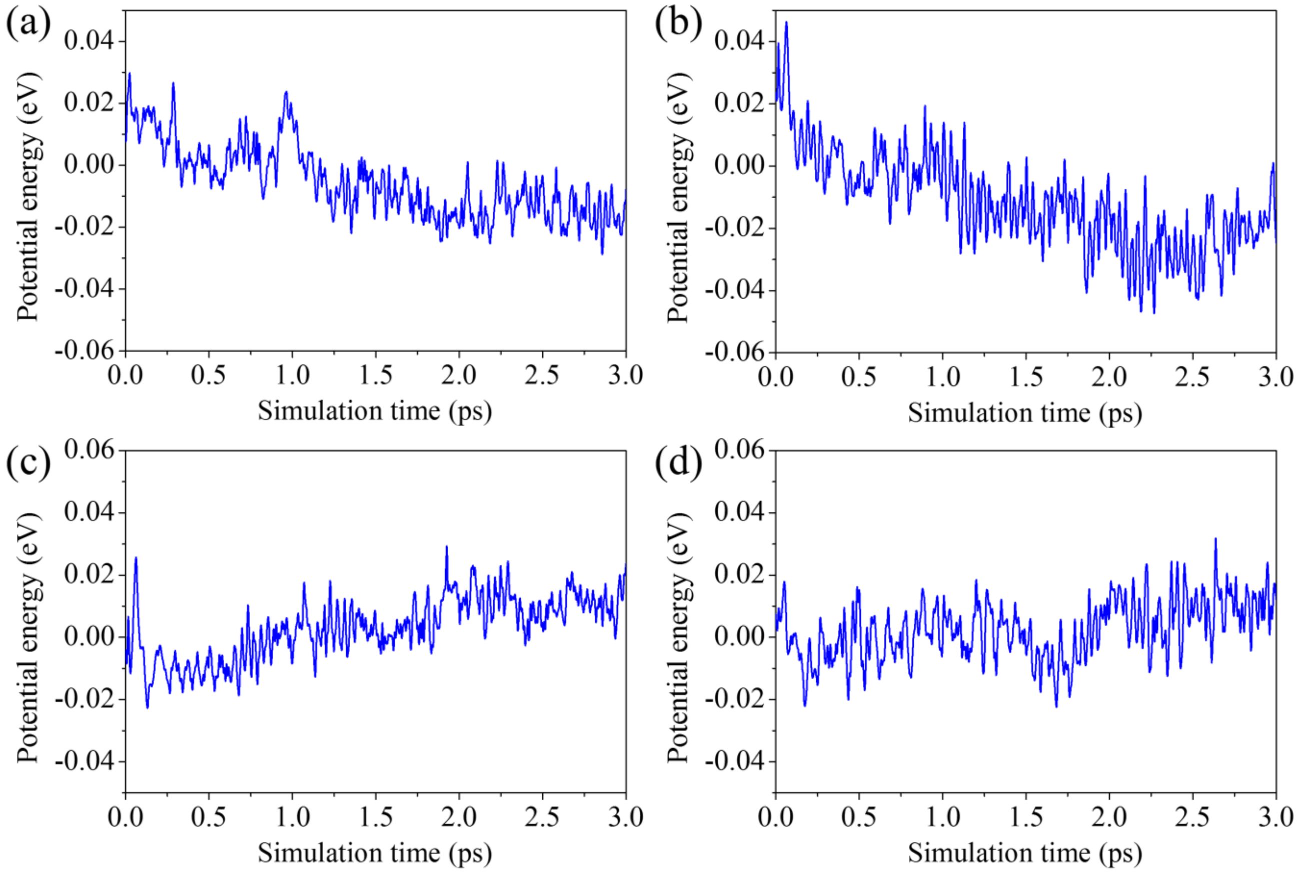

Fig. S1. Constant T simulation of Li_n/BBP (n = 1 ~ 4) using the Nosé-Hoover chain thermostat, with 1.5 fs time step, target temperature 300 K, nose Q ratio = 2.0. (a) ~ (d) show the potential energies of Li/BBP, Li_2/BBP, Li_3/BBP and Li_4/BBP at each time step of the simulation within 3 ps, respectively.

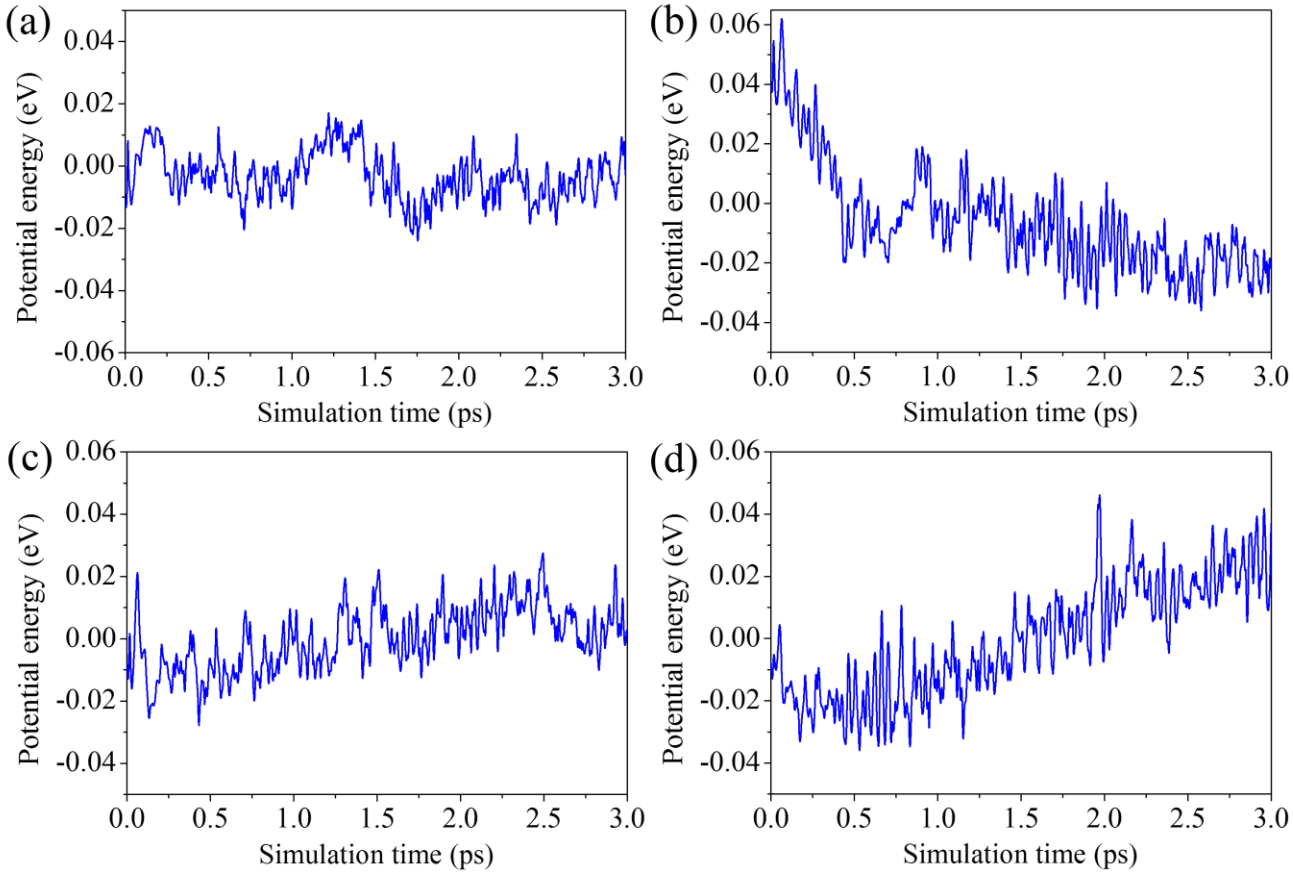

Fig. S2. Constant T simulation of Li_n/BBP (n = 1 ~ 4) under an electric field of 0.25 V $Å^{-1}$ using the Nosé-Hoover chain thermostat, with 1.5 fs time step, target temperature 300 K, nose Q ratio = 2.0. (a) ~ (d) show the potential energies of Li/BBP, Li_2/BBP, Li_3/BBP and Li_4/BBP under an electric field of 0.25 V $Å^{-1}$ at each time step of the simulation within 3 ps, respectively.

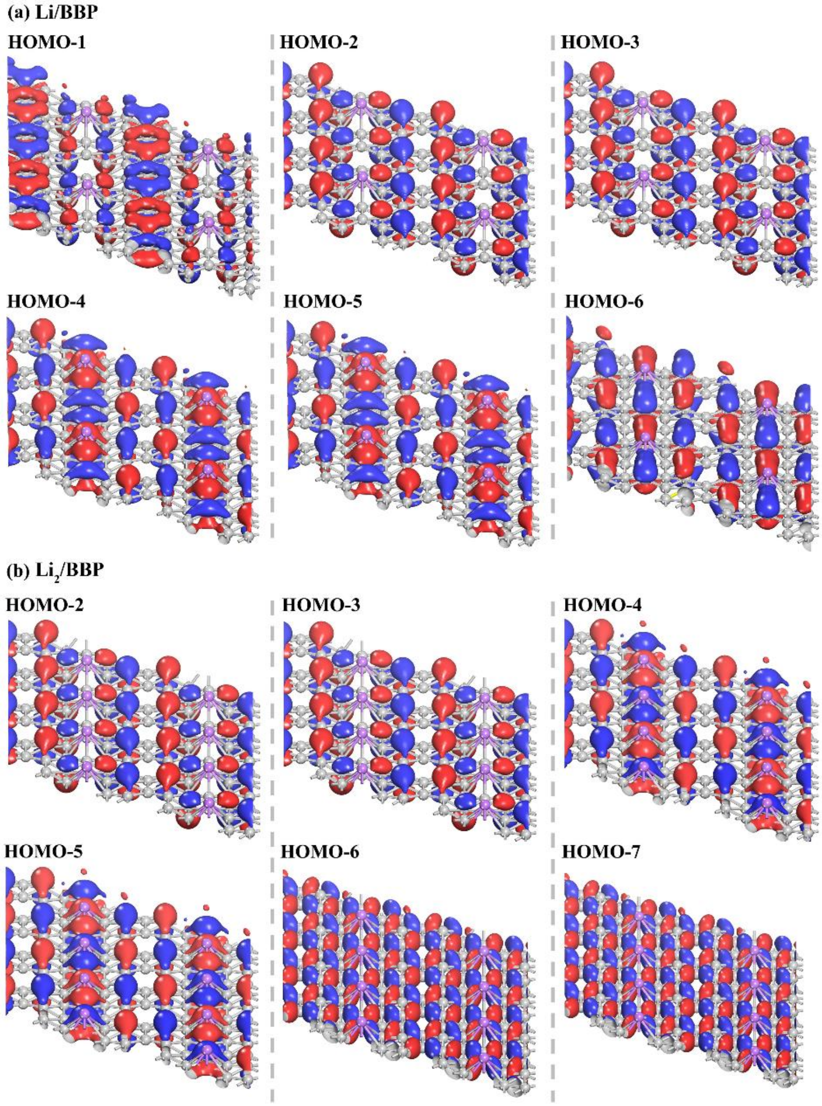

Fig. S3. Schematic images of HOMO-1 ~ HOMO-6 of Li/BBP (a) and HOMO-2 ~ HOMO-7 of Li_2/BBP (b) under an electric field of 0.25 V $Å^{-1}$ and with an isovalue of 0.03 e/A^3.

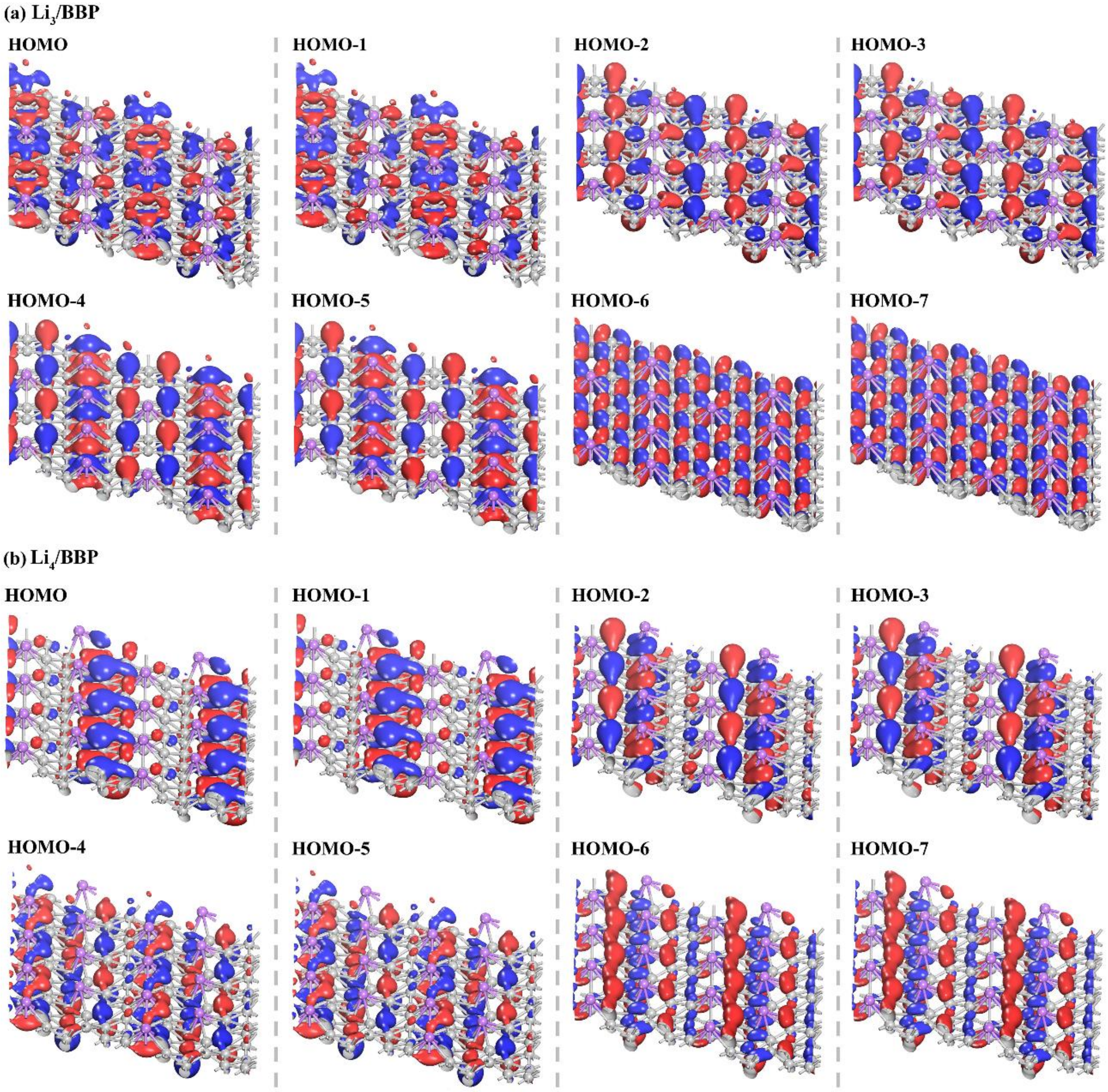

Fig. S4. Schematic images of HOMO ~ HOMO-7 of Li_3/BBP (a) and Li_4/BBP (b) under an electric field of 0.25 V $Å^{-1}$ and with isovalue of 0.03 e/A^3.

Table S1 Optimized average Li-B bond lengths (Å) in Li_n/BBP (n = 1 ~ 4) in the absence and presence of an applied electric field (E, V $Å^{-1}$).

E	Li/BBP	Li_2/BBP	Li_3/BBP	Li_4/BBP
0.00	2.341	2.329	2.309	2.310
0.05	2.341	2.329	2.309	2.310
0.10	2.352	2.329	2.309	2.310
0.15	2.357	2.338	2.317	2.319
0.20	2.364	2.343	2.325	2.324
0.25	2.372	2.352	2.330	2.328

Table S2 Dipole moments (D) of Li_n/BBP, the BBP substrate, and the decorated Li atoms and the induced dipole moment (D) of Li_n/BBP (n = 1 ~ 4) in the presence of an applied electric field (E, V $Å^{-1}$).

Structures	E	Dipole moment			Induced dipole moment (D)
		Li_n/BBP	Li_n	BBP	
Li/BBP	0.00	3.93	0.00	-0.42	4.35
	0.05	4.70	0.00	0.32	4.38
	0.10	5.61	0.00	1.05	4.56
	0.15	6.36	0.00	1.78	4.57
	0.20	7.16	0.00	2.52	4.65
	0.25	8.06	0.00	3.25	4.81
Li_2/BBP	0.00	7.87	0.00	-0.42	8.29
	0.05	8.62	0.00	0.32	8.30
	0.10	9.47	0.00	1.05	8.42
	0.15	10.34	0.00	1.78	8.55
	0.20	11.28	0.00	2.52	8.76
	0.25	12.14	0.00	3.25	8.89
Li_3/BBP	0.00	11.11	0.00	-0.42	11.52
	0.05	11.98	0.00	0.32	11.66
	0.10	12.85	0.00	1.05	11.80
	0.15	13.92	0.00	1.78	12.14
	0.20	14.94	0.00	2.52	12.42
	0.25	15.91	0.00	3.25	12.66
Li_4/BBP	0.00	13.12	0.00	-0.42	13.54
	0.05	14.11	0.00	0.32	13.79
	0.10	15.07	0.00	1.05	14.02
	0.15	16.39	0.00	1.78	14.61
	0.20	17.51	0.00	2.52	15.00
	0.25	18.63	0.00	3.25	15.38

Table S3 Optimized average Li-B bond lengths (in Å) and average bond angles (∠$B_mLi_nB_o$, in degree) in Li_n/BBP (n = 1 ~ 4) before and after MD-NVT simulations (3 ps). B_m and B_o are two o-position boron atoms in a hexagonal hole in BBP, while the Li_n in ∠$B_mLi_nB_o$ is the nth Li atom decorated on the abovementioned hexagonal hole.

	E = 0				E = 0.25 V Å^{-1}			
	Li/BBP	Li_2/BBP	Li_3/BBP	Li_4/BBP	Li/BBP	Li_2/BBP	Li_3/BBP	Li_4/BBP
	Average Li-B bond lengths (in Å)							
Before MD-NVT	2.341	2.329	2.309	2.310	2.372	2.352	2.330	2.328
After MD-NVT	2.313	2.343	2.312	2.337	2.388	2.414	2.364	2.314
Variety	-1.2%	0.6%	0.1%	1.2%	0.7%	2.6%	1.5%	-0.6%
	Average bond angles (∠$B_mLi_nB_o$, in degree)							
Before MD-NVT	42.110	42.373	42.906	43.218	41.575	41.971	42.444	42.772
After MD-NVT	42.370	42.655	43.434	43.608	41.720	41.151	42.838	43.070
Variety	0.6%	0.7%	1.2%	0.9%	0.3%	-2.0%	0.9%	0.7%

Table S4. Emission currents (A) from different orbitals of Li/BBP under different electric fields (V $Å^{-1}$).

Orbitals	Electric fields				
	0.05	0.10	0.15	0.20	0.25
LUMO+10	1.7047E-74	1.9693E-73	0.0000E+00	0.0000E+00	0.0000E+00
LUMO+9	4.3869E-72	4.0269E-72	0.0000E+00	0.0000E+00	0.0000E+00
LUMO+8	1.7405E-63	9.0444E-63	2.1167E-63	0.0000E+00	0.0000E+00
LUMO+7	3.1274E-46	3.4079E-46	4.4027E-47	1.4835E-47	0.0000E+00
LUMO+6	9.4168E-35	6.1512E-36	5.0775E-36	4.6009E-36	4.5063E-36
LUMO+5	2.0519E-29	1.9179E-30	1.8118E-30	1.9001E-30	1.9471E-30
LUMO+4	1.7174E-22	3.6186E-23	2.8521E-23	2.3382E-23	1.8533E-23
LUMO+3	7.7108E-22	4.9768E-22	4.6634E-22	3.6385E-22	3.0600E-22
LUMO+2	2.0348E-15	5.6187E-16	9.0381E-16	9.5967E-16	1.5154E-15
LUMO+1	1.7942E-14	2.5608E-14	1.7540E-14	1.6092E-14	1.6307E-14
LUMO	5.4974E-12	1.2210E-11	1.1630E-11	1.2490E-11	1.1307E-11
HOMO	1.3836E-08	1.4906E-08	1.8261E-08	1.7282E-08	2.0377E-08
HOMO-1	1.1143E-06	1.9841E-06	2.0806E-06	2.0029E-06	3.2244E-06
HOMO-2	1.4644E-06	1.6302E-06	1.6151E-06	1.7166E-06	1.6961E-06
HOMO-3	6.2446E-06	5.9035E-06	5.8164E-06	5.6343E-06	5.5059E-06
HOMO-4	2.2023E-07	2.4380E-07	2.4798E-07	2.3704E-07	1.9808E-07
HOMO-5	8.2137E-07	8.8501E-07	8.7396E-07	8.3937E-07	8.4076E-07
HOMO-6	5.5524E-06	5.2706E-06	5.1705E-06	5.0761E-06	4.9267E-06
HOMO-7	7.6208E-09	6.4250E-09	6.4530E-09	7.3030E-09	5.8384E-09
HOMO-8	7.6555E-08	8.8771E-08	1.1540E-07	9.1004E-08	9.2356E-08
HOMO-9	1.0725E-07	9.4667E-08	9.7539E-08	9.5278E-08	9.4671E-08
HOMO-10	5.4858E-11	5.5177E-11	5.5779E-11	5.6452E-11	5.7457E-11

Table S5. Emission currents (A) from different orbitals of Li_2/BBP under different electric fields (V Å^{-1}).

Orbitals	Electric fields				
	0.05	0.10	0.15	0.20	0.25
LUMO+10	8.6044E-70	3.3126E-70	3.9907E-70	3.8608E-71	0.0000E+00
LUMO+9	7.9569E-52	1.0436E-52	8.0839E-54	6.5753E-55	8.0672E-56
LUMO+8	1.3723E-51	4.1800E-52	9.1174E-52	5.9865E-52	2.1114E-52
LUMO+7	6.5286E-37	5.3021E-37	9.2696E-38	8.4627E-38	3.3563E-37
LUMO+6	1.0108E-34	1.5221E-35	3.9298E-36	9.1876E-37	2.2760E-38
LUMO+5	4.6231E-31	4.4409E-31	7.8340E-32	7.2812E-32	1.0263E-31
LUMO+4	4.0088E-18	2.6707E-18	1.0228E-18	9.9248E-19	8.2024E-19
LUMO+3	4.8305E-18	3.8417E-18	7.8940E-19	5.7616E-19	1.6490E-18
LUMO+2	7.2323E-15	6.8868E-15	9.6482E-16	1.0544E-15	1.0557E-15
LUMO+1	2.9272E-11	1.9132E-11	1.8318E-11	1.8804E-11	1.5721E-11
LUMO	1.6303E-09	1.3397E-09	1.3135E-09	1.4951E-09	1.1349E-09
HOMO	1.0357E-07	9.4505E-08	9.1894E-08	9.1799E-08	9.5127E-08
HOMO-1	3.7072E-08	3.6245E-08	3.9449E-08	3.9216E-08	4.7657E-08
HOMO-2	2.5394E-06	2.5738E-06	4.0730E-06	5.7653E-06	6.7595E-06
HOMO-3	7.1469E-07	7.1336E-07	6.9348E-07	6.9625E-07	6.7917E-07
HOMO-4	5.0351E-06	4.9940E-06	5.0944E-06	5.0592E-06	5.0336E-06
HOMO-5	1.0515E-05	1.0449E-05	1.0048E-05	9.8528E-06	9.7285E-06
HOMO-6	2.1538E-06	2.1571E-06	2.2899E-06	2.3187E-06	2.2892E-06
HOMO-7	1.1585E-05	1.1447E-05	1.1043E-05	1.0952E-05	1.0755E-05
HOMO-8	6.7468E-08	6.7268E-08	6.5827E-08	6.7202E-08	6.7353E-08
HOMO-9	2.3376E-07	2.3306E-07	2.2759E-07	2.2996E-07	2.2454E-07
HOMO-10	1.1243E-07	1.1111E-07	1.1762E-07	1.2329E-07	1.2426E-07

Table S6. Emission currents (A) from different orbitals of Li_3/BBP under different electric fields (V Å^{-1}).

Orbitals	Electric fields				
	0.05	0.10	0.15	0.20	0.25
LUMO+10	1.6962E-57	1.1014E-57	8.7834E-58	6.7705E-58	4.2438E-58
LUMO+9	1.7479E-49	1.2955E-50	4.0470E-51	1.0095E-51	1.6015E-52
LUMO+8	3.8947E-47	3.5398E-48	1.2719E-48	3.1897E-49	5.6841E-50
LUMO+7	2.6204E-43	1.9004E-43	9.3184E-44	8.9692E-44	8.8071E-44
LUMO+6	1.7500E-34	1.6266E-34	2.7309E-34	3.5865E-34	1.3687E-34
LUMO+5	9.3500E-31	9.9457E-31	1.8251E-30	2.9545E-30	2.1986E-32
LUMO+4	5.9811E-25	1.3521E-25	8.3464E-26	4.6817E-26	1.7974E-26
LUMO+3	5.7951E-18	5.1388E-18	2.8891E-17	3.8712E-17	4.5964E-17
LUMO+2	6.3328E-15	5.3258E-15	8.6094E-15	8.7311E-15	8.7558E-15
LUMO+1	1.3763E-11	1.2357E-11	1.9815E-11	1.9078E-11	1.9710E-11
LUMO	7.6957E-08	7.5318E-08	7.1761E-08	9.8967E-08	1.0365E-07
HOMO	2.5718E-07	2.4885E-07	2.6567E-07	3.4428E-07	3.4489E-07
HOMO-1	8.8100E-07	8.6954E-07	9.9788E-07	1.0198E-06	1.0426E-06
HOMO-2	4.7691E-06	4.7182E-06	5.3185E-06	5.9569E-06	6.2855E-06
HOMO-3	9.1088E-07	9.0780E-07	8.9600E-07	9.9126E-07	9.5603E-07
HOMO-4	1.2236E-05	1.2165E-05	1.2036E-05	1.2065E-05	1.1976E-05
HOMO-5	7.4357E-06	7.4075E-06	9.6047E-06	9.7996E-06	1.0575E-05
HOMO-6	3.7990E-06	3.8250E-06	3.9798E-06	3.9486E-06	3.9071E-06
HOMO-7	9.7685E-06	9.7251E-06	9.9509E-06	9.4293E-06	9.3586E-06
HOMO-8	2.0501E-07	2.0466E-07	1.9838E-07	1.9570E-07	1.5505E-07
HOMO-9	8.7209E-08	8.6867E-08	1.0455E-07	1.0337E-07	1.0432E-07
HOMO-10	1.5937E-07	1.5899E-07	1.6105E-07	1.6209E-07	1.6296E-07

Table S7. Emission currents (A) from different orbitals of Li_4/BBP under different electric fields (V Å^{-1}).

Orbitals	Electric fields				
	0.05	0.10	0.15	0.20	0.25
LUMO+10	3.2411E-58	8.10E-61	5.3051E-59	1.8645E-59	6.9067E-60
LUMO+9	7.5600E-53	5.80E-59	5.7639E-53	7.1591E-53	9.2426E-53
LUMO+8	4.0978E-48	3.26E-53	6.9143E-49	3.3611E-49	1.7425E-49
LUMO+7	4.7147E-48	1.75E-48	1.4473E-47	6.1208E-48	9.8947E-48
LUMO+6	1.0297E-45	4.91E-48	2.3348E-45	7.8703E-46	1.3397E-45
LUMO+5	9.1083E-34	6.45E-46	2.8165E-34	1.6185E-34	8.4708E-35
LUMO+4	7.3066E-26	2.39E-34	3.7782E-26	7.9322E-26	1.1112E-25
LUMO+3	7.7926E-18	6.26E-26	8.8154E-18	1.0267E-17	1.0949E-17
LUMO+2	8.7461E-08	6.91E-18	1.2760E-07	1.0175E-07	7.6964E-08
LUMO+1	4.3027E-07	8.85E-08	5.1842E-07	6.3943E-07	6.9156E-07
LUMO	1.7255E-07	4.18E-07	5.0503E-07	6.4591E-07	7.3261E-07
HOMO	3.2453E-06	1.69E-07	3.2791E-06	4.0966E-06	5.0615E-06
HOMO-1	3.3044E-06	3.23E-06	3.3041E-06	4.8558E-06	5.6235E-06
HOMO-2	6.6836E-06	3.2763E-06	6.9478E-06	6.9627E-06	7.1742E-06
HOMO-3	2.8056E-06	6.5805E-06	2.7951E-06	2.8738E-06	3.0601E-06
HOMO-4	6.7594E-06	2.7952E-06	8.2835E-06	7.9310E-06	7.8261E-06
HOMO-5	1.8351E-06	6.7279E-06	2.2139E-06	2.2732E-06	2.1752E-06
HOMO-6	7.3278E-06	1.8351E-06	7.1473E-06	7.0893E-06	7.0500E-06
HOMO-7	1.0555E-05	7.3055E-06	1.0380E-05	1.0088E-05	9.9106E-06
HOMO-8	6.5002E-07	1.0506E-05	5.8670E-07	5.2480E-07	5.1875E-07
HOMO-9	4.6079E-07	6.5134E-07	4.3114E-07	4.3059E-07	4.2618E-07
HOMO-10	4.5890E-07	4.6120E-07	3.5803E-07	4.0549E-07	4.0716E-07

Structure data S1. Optimized geometries of Li_n/BBP in the absence of an applied electric field.

Li/BBP without an applied electric field

B	0.49454	0.97488	0.00736
B	0.99428	0.47478	-0.01058
B	0.32899	0.64063	-0.00030
B	0.32926	0.14063	-0.00226
B	0.66033	0.14063	-0.00226
B	0.49505	0.30638	0.00736
B	0.32836	0.80675	-0.00977
B	0.82878	0.30638	0.00736
B	0.16114	0.47478	-0.01058
B	0.66122	0.47450	-0.00977
B	0.16002	0.64063	0.00052
B	0.99530	0.80647	-0.01058
B	0.32844	0.30690	0.00639
B	0.16080	0.97488	0.00736
B	0.49449	0.47450	-0.00977
B	0.82957	0.64063	0.00052
B	0.82844	0.80647	-0.01058
B	0.66115	0.97435	0.00639
B	0.99471	0.97435	0.00639
B	0.82926	0.14063	-0.00226
B	0.66059	0.64063	-0.00030
B	0.16032	0.14063	-0.00226
B	0.49510	0.80675	-0.00977
B	0.99487	0.30690	0.00639
B	0.32843	0.97336	0.01531
B	0.32819	0.47209	-0.01951
B	0.82859	0.97304	0.01420
B	0.66116	0.30790	0.01531
B	0.82993	0.47209	-0.01951
B	0.66140	0.80916	-0.01951
B	0.16100	0.30822	0.01420
B	0.15965	0.80916	-0.01951
Li	0.49479	0.64063	0.09528

Li_2/BBP without an applied electric field

B	0.49472	0.97484	0.00720
B	0.99405	0.47503	-0.01065
B	0.32898	0.64063	0.00301
B	0.32940	0.14063	-0.00272
B	0.66018	0.14063	-0.00272
B	0.49486	0.30641	0.00720
B	0.32845	0.80622	-0.01065
B	0.82894	0.30641	0.00720
B	0.16113	0.47503	-0.01065
B	0.66113	0.47503	-0.01065
B	0.16060	0.64063	0.00301
B	0.99554	0.80622	-0.01065
B	0.32894	0.30641	0.00720
B	0.16065	0.97484	0.00720
B	0.49405	0.47503	-0.01065
B	0.82898	0.64063	0.00301
B	0.82845	0.80622	-0.01065
B	0.66065	0.97484	0.00720
B	0.99472	0.97484	0.00720
B	0.82940	0.14063	-0.00272
B	0.66060	0.64063	0.00301
B	0.16018	0.14063	-0.00272
B	0.49554	0.80622	-0.01065
B	0.99486	0.30641	0.00720
B	0.32824	0.97373	0.01496
B	0.32941	0.47139	-0.02178
B	0.82824	0.97373	0.01496
B	0.66134	0.30753	0.01496
B	0.82941	0.47139	-0.02178
B	0.66017	0.80986	-0.02178
B	0.16134	0.30753	0.01496
B	0.16017	0.80986	-0.02178
Li	0.99479	0.64063	0.09477
Li	0.49479	0.64063	0.09477

Li_3/BBP without an applied electric field

B	0.49466	0.97402	0.01189
B	0.99356	0.47477	-0.01388
B	0.32906	0.64050	-0.00099
B	0.32997	0.14063	0.00153
B	0.65961	0.14063	0.00153
B	0.49493	0.30723	0.01189
B	0.32770	0.80649	-0.01388
B	0.82777	0.30803	0.01309
B	0.16207	0.47347	-0.01497
B	0.66189	0.47477	-0.01388
B	0.16065	0.64050	-0.00099
B	0.99602	0.80649	-0.01388
B	0.32805	0.30723	0.01189
B	0.16182	0.97323	0.01309
B	0.49467	0.47347	-0.01497
B	0.82894	0.64075	-0.00099
B	0.82751	0.80778	-0.01497
B	0.66153	0.97402	0.01189
B	0.99516	0.97323	0.01309
B	0.82991	0.14063	0.00018
B	0.66052	0.64075	-0.00099
B	0.15968	0.14063	0.00018
B	0.49492	0.80778	-0.01497
B	0.99442	0.30803	0.01309
B	0.32947	0.97248	0.01971
B	0.32968	0.47086	-0.02443
B	0.82826	0.97248	0.01971
B	0.66012	0.30877	0.01971
B	0.82966	0.47089	-0.02852
B	0.65991	0.81040	-0.02443
B	0.16132	0.30877	0.01971
B	0.15992	0.81036	-0.02852
Li	0.99479	0.64063	0.08809
Li	0.49479	0.64063	0.08809
Li	0.99479	0.14063	0.10870

Li_4/BBP without an applied electric field

B	0.49458	0.97079	0.02317
B	0.99433	0.47045	-0.03490
B	0.32911	0.63602	-0.00855
B	0.32858	0.13853	0.00108
B	0.65848	0.13855	0.00111
B	0.49388	0.30824	0.00596
B	0.33050	0.79904	0.01514
B	0.82350	0.30820	0.00591
B	0.16083	0.47043	-0.03488
B	0.66083	0.47043	-0.03488
B	0.16047	0.63600	-0.00851
B	0.99604	0.79904	0.01519
B	0.32350	0.30820	0.00591
B	0.16024	0.97078	0.02314
B	0.49433	0.47045	-0.03490
B	0.82911	0.63602	-0.00855
B	0.83050	0.79904	0.01514
B	0.66024	0.97078	0.02314
B	0.99458	0.97079	0.02317
B	0.82858	0.13853	0.00108
B	0.66047	0.63600	-0.00851
B	0.15848	0.13855	0.00111
B	0.49604	0.79904	0.01519
B	0.99388	0.30824	0.00596
B	0.32628	0.97306	0.00121
B	0.32901	0.46759	-0.04085
B	0.82628	0.97306	0.00121
B	0.65521	0.31516	0.02484
B	0.82901	0.46759	-0.04085
B	0.66081	0.80396	-0.00725
B	0.15521	0.31516	0.02484
B	0.16081	0.80396	-0.00725
Li	1.01970	0.58615	0.08438
Li	0.51970	0.58615	0.08438
Li	0.98472	0.15613	0.10771
Li	0.48472	0.15613	0.10771

Structure data S2. Optimized geometries of Li_n /BBP in the presence of an applied electric field (E, V Å^{-1}).

Li/BBP under an applied electric field of 0.05 V Å^{-1}

B	0.49453	0.97488	0.00736
B	0.99428	0.47479	-0.01060
B	0.32899	0.64063	-0.00023
B	0.32926	0.14063	-0.00230
B	0.66033	0.14062	-0.00230
B	0.49505	0.30638	0.00736
B	0.32836	0.80674	-0.00976
B	0.82878	0.30638	0.00736
B	0.16115	0.47479	-0.01060
B	0.66122	0.47451	-0.00976
B	0.16002	0.64062	0.00058
B	0.99530	0.80647	-0.01060
B	0.32843	0.30690	0.00638
B	0.16081	0.97488	0.00736
B	0.49448	0.47451	-0.00976
B	0.82956	0.64063	0.00058
B	0.82844	0.80647	-0.01060
B	0.66115	0.97435	0.00638
B	0.99471	0.97435	0.00638
B	0.82926	0.14063	-0.00229
B	0.66059	0.64063	-0.00023
B	0.16033	0.14063	-0.00229
B	0.49510	0.80675	-0.00976
B	0.99487	0.30690	0.00638
B	0.32842	0.97336	0.01532
B	0.32818	0.47210	-0.01953
B	0.82858	0.97305	0.01419
B	0.66116	0.30789	0.01532
B	0.82993	0.47210	-0.01953
B	0.66140	0.80916	-0.01953
B	0.16100	0.30821	0.01419
B	0.15966	0.80916	-0.01953
Li	0.49479	0.64063	0.09532

Li/BBP under an applied electric field of 0.10 V Å^{-1}

B	0.49450	0.97485	0.00714
B	0.99414	0.47492	-0.01089
B	0.32893	0.64065	0.00153
B	0.32930	0.14066	-0.00299
B	0.66029	0.14060	-0.00299
B	0.49508	0.30640	0.00714
B	0.32829	0.80667	-0.00970
B	0.82873	0.30637	0.00724
B	0.16113	0.47496	-0.01092
B	0.66130	0.47458	-0.00970
B	0.16007	0.64061	0.00185
B	0.99544	0.80634	-0.01089
B	0.32836	0.30694	0.00615
B	0.16085	0.97488	0.00724
B	0.49436	0.47455	-0.00967
B	0.82952	0.64064	0.00185
B	0.82845	0.80629	-0.01092
B	0.66122	0.97431	0.00615
B	0.99469	0.97429	0.00611
B	0.82931	0.14063	-0.00296
B	0.66066	0.64060	0.00153
B	0.16028	0.14062	-0.00296
B	0.49523	0.80670	-0.00967
B	0.99490	0.30697	0.00611
B	0.32836	0.97339	0.01543
B	0.32805	0.47225	-0.02013
B	0.82846	0.97316	0.01406
B	0.66122	0.30786	0.01543
B	0.82984	0.47222	-0.02010
B	0.66153	0.80900	-0.02013
B	0.16112	0.30810	0.01406
B	0.15975	0.80904	-0.02010
Li	0.49479	0.64063	0.09689

Li/BBP under an applied electric field of 0.15 V Å^{-1}

B	0.49448	0.97487	0.00708
B	0.99415	0.47490	-0.01109
B	0.32892	0.64066	0.00181
B	0.32931	0.14065	-0.00316
B	0.66027	0.14061	-0.00316
B	0.49511	0.30638	0.00708
B	0.32835	0.80659	-0.00946
B	0.82871	0.30636	0.00719
B	0.16115	0.47494	-0.01114
B	0.66123	0.47466	-0.00946
B	0.16004	0.64060	0.00183
B	0.99543	0.80635	-0.01109
B	0.32837	0.30691	0.00600
B	0.16087	0.97489	0.00719
B	0.49435	0.47463	-0.00942
B	0.82955	0.64066	0.00183
B	0.82843	0.80632	-0.01114
B	0.66121	0.97435	0.00600
B	0.99467	0.97432	0.00595
B	0.82929	0.14066	-0.00312
B	0.66066	0.64060	0.00181
B	0.16029	0.14059	-0.00312
B	0.49524	0.80663	-0.00942
B	0.99492	0.30693	0.00595
B	0.32834	0.97343	0.01553
B	0.32807	0.47229	-0.02008
B	0.82844	0.97317	0.01394
B	0.66124	0.30783	0.01553
B	0.82976	0.47227	-0.02004
B	0.66152	0.80896	-0.02008
B	0.16114	0.30808	0.01394
B	0.15982	0.80899	-0.02004
Li	0.49479	0.64063	0.09760

Li/BBP under an applied electric field of 0.20 V Å^{-1}

B	0.49449	0.97487	0.00709
B	0.99414	0.47494	-0.01098
B	0.32891	0.64064	0.00166
B	0.32929	0.14065	-0.00303
B	0.66029	0.14060	-0.00303
B	0.49509	0.30639	0.00709
B	0.32827	0.80671	-0.00969
B	0.82875	0.30636	0.00715
B	0.16111	0.47497	-0.01099
B	0.66131	0.47455	-0.00969
B	0.16009	0.64061	0.00173
B	0.99545	0.80632	-0.01098
B	0.32835	0.30696	0.00609
B	0.16084	0.97489	0.00715
B	0.49437	0.47452	-0.00967
B	0.82949	0.64064	0.00173
B	0.82847	0.80628	-0.01099
B	0.66124	0.97430	0.00609
B	0.99468	0.97428	0.00606
B	0.82931	0.14062	-0.00301
B	0.66067	0.64062	0.00166
B	0.16027	0.14064	-0.00301
B	0.49522	0.80673	-0.00967
B	0.99490	0.30698	0.00606
B	0.32838	0.97338	0.01552
B	0.32811	0.47222	-0.02015
B	0.82850	0.97312	0.01397
B	0.66120	0.30788	0.01552
B	0.82983	0.47220	-0.02011
B	0.66147	0.80903	-0.02015
B	0.16108	0.30814	0.01397
B	0.15975	0.80905	-0.02011
Li	0.49479	0.64063	0.09798

Li/BBP under an applied electric field of 0.25 V Å^{-1}

B	0.49446	0.97491	0.00702
B	0.99411	0.47495	-0.01098
B	0.32898	0.64063	0.00166
B	0.32926	0.14069	-0.00306
B	0.66032	0.14057	-0.00306
B	0.49512	0.30634	0.00702
B	0.32828	0.80673	-0.00976
B	0.82874	0.30634	0.00706
B	0.16114	0.47497	-0.01099
B	0.66130	0.47453	-0.00976
B	0.16018	0.64061	0.00174
B	0.99547	0.80630	-0.01098
B	0.32834	0.30697	0.00611
B	0.16084	0.97492	0.00706
B	0.49439	0.47451	-0.00973
B	0.82941	0.64065	0.00174
B	0.82845	0.80629	-0.01099
B	0.66124	0.97428	0.00611
B	0.99469	0.97427	0.00608
B	0.82931	0.14059	-0.00304
B	0.66060	0.64063	0.00166
B	0.16028	0.14066	-0.00304
B	0.49519	0.80675	-0.00973
B	0.99489	0.30699	0.00608
B	0.32840	0.97337	0.01550
B	0.32818	0.47221	-0.02015
B	0.82853	0.97309	0.01392
B	0.66119	0.30788	0.01550
B	0.82979	0.47220	-0.02011
B	0.66141	0.80904	-0.02015
B	0.16106	0.30816	0.01392
B	0.15979	0.80905	-0.02011
Li	0.49479	0.64063	0.09866

Li_2/BBP under an applied electric field of 0.05 V $Å^{-1}$

B	0.49472	0.97484	0.00720
B	0.99404	0.47503	-0.01066
B	0.32898	0.64063	0.00305
B	0.32940	0.14063	-0.00273
B	0.66018	0.14062	-0.00273
B	0.49487	0.30641	0.00720
B	0.32845	0.80622	-0.01066
B	0.82893	0.30641	0.00720
B	0.16113	0.47504	-0.01066
B	0.66113	0.47504	-0.01066
B	0.16060	0.64062	0.00305
B	0.99554	0.80622	-0.01066
B	0.32893	0.30641	0.00720
B	0.16065	0.97484	0.00720
B	0.49404	0.47503	-0.01066
B	0.82898	0.64063	0.00305
B	0.82845	0.80622	-0.01066
B	0.66065	0.97484	0.00720
B	0.99472	0.97484	0.00720
B	0.82940	0.14063	-0.00273
B	0.66060	0.64062	0.00305
B	0.16018	0.14062	-0.00273
B	0.49554	0.80622	-0.01066
B	0.99487	0.30641	0.00720
B	0.32824	0.97373	0.01496
B	0.32940	0.47140	-0.02180
B	0.82824	0.97373	0.01496
B	0.66134	0.30753	0.01496
B	0.82940	0.47140	-0.02180
B	0.66018	0.80986	-0.02180
B	0.16134	0.30753	0.01496
B	0.16018	0.80986	-0.02180
Li	0.99479	0.64063	0.09478
Li	0.49479	0.64063	0.09478

Li_2/BBP under an applied electric field of 0.10 V $Å^{-1}$

B	0.49472	0.97484	0.00719
B	0.99404	0.47504	-0.01065
B	0.32898	0.64063	0.00305
B	0.32940	0.14063	-0.00275
B	0.66018	0.14062	-0.00275
B	0.49487	0.30641	0.00719
B	0.32845	0.80621	-0.01065
B	0.82893	0.30641	0.00720
B	0.16113	0.47504	-0.01065
B	0.66113	0.47504	-0.01065
B	0.16060	0.64062	0.00305
B	0.99554	0.80621	-0.01065
B	0.32893	0.30641	0.00720
B	0.16065	0.97484	0.00720
B	0.49404	0.47504	-0.01065
B	0.82898	0.64063	0.00305
B	0.82845	0.80621	-0.01065
B	0.66065	0.97484	0.00720
B	0.99472	0.97484	0.00719
B	0.82940	0.14063	-0.00275
B	0.66060	0.64062	0.00305
B	0.16018	0.14062	-0.00275
B	0.49554	0.80621	-0.01065
B	0.99487	0.30641	0.00719
B	0.32824	0.97373	0.01495
B	0.32940	0.47140	-0.02179
B	0.82824	0.97373	0.01495
B	0.66135	0.30752	0.01495
B	0.82940	0.47140	-0.02179
B	0.66018	0.80985	-0.02179
B	0.16135	0.30752	0.01495
B	0.16018	0.80985	-0.02179
Li	0.99479	0.64063	0.09480
Li	0.49479	0.64063	0.09480

Li_2/BBP under an applied electric field of 0.15 V Å^{-1}

B	0.49467	0.97480	0.00719
B	0.99395	0.47505	-0.01091
B	0.32894	0.64064	0.00383
B	0.32947	0.14064	-0.00309
B	0.66011	0.14062	-0.00309
B	0.49492	0.30646	0.00719
B	0.32838	0.80617	-0.01092
B	0.82886	0.30643	0.00722
B	0.16120	0.47509	-0.01092
B	0.66120	0.47509	-0.01092
B	0.16064	0.64062	0.00383
B	0.99563	0.80621	-0.01091
B	0.32886	0.30643	0.00722
B	0.16072	0.97483	0.00722
B	0.49395	0.47505	-0.01091
B	0.82894	0.64064	0.00383
B	0.82838	0.80617	-0.01092
B	0.66072	0.97483	0.00722
B	0.99467	0.97480	0.00719
B	0.82947	0.14064	-0.00309
B	0.66064	0.64062	0.00383
B	0.16011	0.14062	-0.00309
B	0.49563	0.80621	-0.01091
B	0.99492	0.30646	0.00719
B	0.32818	0.97379	0.01492
B	0.32931	0.47156	-0.02213
B	0.82818	0.97379	0.01492
B	0.66140	0.30746	0.01492
B	0.82931	0.47156	-0.02213
B	0.66027	0.80970	-0.02213
B	0.16140	0.30746	0.01492
B	0.16027	0.80970	-0.02213
Li	0.99479	0.64063	0.09565
Li	0.49479	0.64063	0.09565

Li_2/BBP under an applied electric field of 0.20V $Å^{-1}$

B	0.49464	0.97483	0.00701
B	0.99393	0.47512	-0.01082
B	0.32894	0.64064	0.00407
B	0.32948	0.14064	-0.00339
B	0.66010	0.14061	-0.00339
B	0.49494	0.30643	0.00701
B	0.32843	0.80609	-0.01083
B	0.82887	0.30639	0.00704
B	0.16115	0.47516	-0.01083
B	0.66115	0.47516	-0.01083
B	0.16064	0.64061	0.00407
B	0.99565	0.80614	-0.01082
B	0.32887	0.30639	0.00704
B	0.16072	0.97486	0.00704
B	0.49393	0.47512	-0.01082
B	0.82894	0.64064	0.00407
B	0.82843	0.80609	-0.01083
B	0.66072	0.97486	0.00704
B	0.99464	0.97483	0.00701
B	0.82948	0.14064	-0.00339
B	0.66064	0.64061	0.00407
B	0.16010	0.14061	-0.00339
B	0.49565	0.80614	-0.01082
B	0.99494	0.30643	0.00701
B	0.32815	0.97384	0.01479
B	0.32926	0.47165	-0.02206
B	0.82815	0.97384	0.01479
B	0.66143	0.30741	0.01479
B	0.82926	0.47165	-0.02206
B	0.66032	0.80960	-0.02206
B	0.16143	0.30741	0.01479
B	0.16032	0.80960	-0.02206
Li	0.99479	0.64063	0.09628
Li	0.49479	0.64063	0.09628

Li_2/BBP under an applied electric field of 0.25 V Å^{-1}

B	0.49466	0.97481	0.00702
B	0.99398	0.47503	-0.01099
B	0.32902	0.64063	0.00387
B	0.32947	0.14063	-0.00324
B	0.66012	0.14062	-0.00324
B	0.49493	0.30644	0.00702
B	0.32840	0.80620	-0.01099
B	0.82885	0.30643	0.00704
B	0.16119	0.47506	-0.01099
B	0.66119	0.47506	-0.01099
B	0.16057	0.64062	0.00387
B	0.99561	0.80623	-0.01099
B	0.32885	0.30643	0.00704
B	0.16073	0.97483	0.00704
B	0.49398	0.47503	-0.01099
B	0.82902	0.64063	0.00387
B	0.82840	0.80620	-0.01099
B	0.66073	0.97483	0.00704
B	0.99466	0.97481	0.00702
B	0.82947	0.14063	-0.00324
B	0.66057	0.64062	0.00387
B	0.16012	0.14062	-0.00324
B	0.49561	0.80623	-0.01099
B	0.99493	0.30644	0.00702
B	0.32819	0.97379	0.01484
B	0.32931	0.47156	-0.02202
B	0.82819	0.97379	0.01484
B	0.66139	0.30746	0.01484
B	0.82931	0.47156	-0.02202
B	0.66027	0.80969	-0.02202
B	0.16139	0.30746	0.01484
B	0.16027	0.80969	-0.02202
Li	0.99479	0.64063	0.09685
Li	0.49479	0.64063	0.09685

Li_3/BBP under an applied electric field of 0.05 V $Å^{-1}$

B	0.49464	0.97403	0.01186
B	0.99356	0.47478	-0.01387
B	0.32906	0.64050	-0.00096
B	0.32997	0.14062	0.00148
B	0.65962	0.14063	0.00148
B	0.49494	0.30722	0.01186
B	0.32770	0.80648	-0.01386
B	0.82778	0.30801	0.01306
B	0.16206	0.47349	-0.01494
B	0.66188	0.47478	-0.01386
B	0.16064	0.64050	-0.00096
B	0.99603	0.80648	-0.01387
B	0.32806	0.30722	0.01185
B	0.16180	0.97324	0.01306
B	0.49467	0.47349	-0.01494
B	0.82894	0.64075	-0.00096
B	0.82752	0.80777	-0.01494
B	0.66153	0.97404	0.01185
B	0.99516	0.97324	0.01307
B	0.82992	0.14062	0.00015
B	0.66052	0.64075	-0.00096
B	0.15966	0.14063	0.00015
B	0.49492	0.80777	-0.01494
B	0.99442	0.30802	0.01307
B	0.32946	0.97248	0.01970
B	0.32968	0.47087	-0.02440
B	0.82827	0.97248	0.01970
B	0.66012	0.30877	0.01970
B	0.82966	0.47090	-0.02851
B	0.65991	0.81039	-0.02440
B	0.16131	0.30877	0.01970
B	0.15993	0.81035	-0.02851
Li	0.99479	0.64063	0.08812
Li	0.49479	0.64063	0.08813
Li	0.99479	0.14063	0.10869

Li_3/BBP under an applied electric field of 0.10 V $Å^{-1}$

B	0.49464	0.97404	0.01185
B	0.99356	0.47478	-0.01386
B	0.32907	0.64050	-0.00095
B	0.32996	0.14062	0.00147
B	0.65962	0.14063	0.00147
B	0.49494	0.30722	0.01185
B	0.32771	0.80648	-0.01386
B	0.82779	0.30801	0.01306
B	0.16206	0.47349	-0.01494
B	0.66188	0.47478	-0.01386
B	0.16064	0.64050	-0.00096
B	0.99603	0.80648	-0.01386
B	0.32806	0.30721	0.01184
B	0.16180	0.97325	0.01306
B	0.49467	0.47349	-0.01494
B	0.82894	0.64075	-0.00096
B	0.82753	0.80776	-0.01494
B	0.66153	0.97404	0.01184
B	0.99516	0.97324	0.01307
B	0.82993	0.14062	0.00015
B	0.66052	0.64076	-0.00095
B	0.15965	0.14063	0.00015
B	0.49492	0.80776	-0.01494
B	0.99442	0.30801	0.01307
B	0.32946	0.97249	0.01970
B	0.32968	0.47087	-0.02440
B	0.82827	0.97249	0.01970
B	0.66013	0.30877	0.01970
B	0.82966	0.47091	-0.02850
B	0.65991	0.81038	-0.02440
B	0.16131	0.30877	0.01970
B	0.15993	0.81035	-0.02850
Li	0.99479	0.64063	0.08814
Li	0.49479	0.64063	0.08814
Li	0.99479	0.14063	0.10870

Li_3/BBP under an applied electric field of 0.15 V Å^{-1}

B	0.49456	0.97417	0.01133
B	0.99357	0.47493	-0.01360
B	0.32910	0.64050	-0.00055
B	0.32999	0.14060	0.00082
B	0.65960	0.14065	0.00082
B	0.49503	0.30709	0.01133
B	0.32787	0.80634	-0.01352
B	0.82799	0.30765	0.01244
B	0.16182	0.47374	-0.01463
B	0.66172	0.47491	-0.01352
B	0.16058	0.64053	-0.00063
B	0.99601	0.80633	-0.01360
B	0.32814	0.30705	0.01123
B	0.16159	0.97361	0.01244
B	0.49462	0.47378	-0.01460
B	0.82900	0.64072	-0.00063
B	0.82777	0.80752	-0.01463
B	0.66145	0.97420	0.01123
B	0.99499	0.97358	0.01259
B	0.83002	0.14060	-0.00042
B	0.66049	0.64075	-0.00055
B	0.15957	0.14066	-0.00042
B	0.49497	0.80747	-0.01460
B	0.99460	0.30767	0.01259
B	0.32940	0.97258	0.01934
B	0.32965	0.47101	-0.02389
B	0.82831	0.97259	0.01937
B	0.66018	0.30867	0.01934
B	0.82963	0.47106	-0.02813
B	0.65993	0.81025	-0.02389
B	0.16127	0.30866	0.01937
B	0.15996	0.81019	-0.02813
Li	0.99479	0.64063	0.08930
Li	0.49479	0.64063	0.08938
Li	0.99479	0.14063	0.10889

Li_3/BBP under an applied electric field of 0.20 V Å^{-1}

B	0.49459	0.97414	0.01145
B	0.99359	0.47485	-0.01372
B	0.32914	0.64052	-0.00079
B	0.33002	0.14062	0.00107
B	0.65956	0.14063	0.00107
B	0.49499	0.30712	0.01145
B	0.32781	0.80642	-0.01367
B	0.82802	0.30772	0.01237
B	0.16191	0.47360	-0.01477
B	0.66178	0.47484	-0.01367
B	0.16055	0.64053	-0.00082
B	0.99599	0.80640	-0.01372
B	0.32810	0.30711	0.01140
B	0.16156	0.97354	0.01237
B	0.49468	0.47362	-0.01478
B	0.82903	0.64073	-0.00082
B	0.82768	0.80765	-0.01477
B	0.66148	0.97415	0.01140
B	0.99510	0.97353	0.01248
B	0.82993	0.14062	-0.00049
B	0.66045	0.64074	-0.00079
B	0.15965	0.14064	-0.00049
B	0.49491	0.80763	-0.01478
B	0.99448	0.30772	0.01248
B	0.32936	0.97258	0.01921
B	0.32967	0.47091	-0.02390
B	0.82834	0.97258	0.01928
B	0.66022	0.30867	0.01921
B	0.82962	0.47103	-0.02811
B	0.65991	0.81035	-0.02390
B	0.16125	0.30868	0.01928
B	0.15996	0.81023	-0.02811
Li	0.99479	0.64063	0.08987
Li	0.49479	0.64063	0.08991
Li	0.99479	0.14063	0.10961

Li_3/BBP under an applied electric field of 0.25 V Å^{-1}

B	0.49459	0.97415	0.01134
B	0.99359	0.47487	-0.01368
B	0.32916	0.64051	-0.00076
B	0.33004	0.14062	0.00095
B	0.65954	0.14064	0.00095
B	0.49499	0.30710	0.01134
B	0.32783	0.80640	-0.01363
B	0.82807	0.30766	0.01228
B	0.16188	0.47363	-0.01476
B	0.66176	0.47485	-0.01363
B	0.16054	0.64052	-0.00080
B	0.99599	0.80638	-0.01368
B	0.32811	0.30709	0.01129
B	0.16152	0.97360	0.01228
B	0.49467	0.47365	-0.01477
B	0.82904	0.64073	-0.00080
B	0.82770	0.80762	-0.01476
B	0.66147	0.97417	0.01129
B	0.99509	0.97359	0.01239
B	0.82994	0.14062	-0.00059
B	0.66043	0.64074	-0.00076
B	0.15965	0.14064	-0.00059
B	0.49491	0.80761	-0.01477
B	0.99450	0.30766	0.01239
B	0.32935	0.97261	0.01907
B	0.32966	0.47093	-0.02387
B	0.82832	0.97261	0.01914
B	0.66023	0.30864	0.01907
B	0.82961	0.47105	-0.02806
B	0.65993	0.81032	-0.02387
B	0.16126	0.30865	0.01914
B	0.15997	0.81021	-0.02806
Li	0.99479	0.64063	0.09034
Li	0.49479	0.64063	0.09038
Li	0.99479	0.14063	0.11003

Li_4/BBP under an applied electric field of 0.05 V $Å^{-1}$

B	0.49459	0.97079	0.02313
B	0.99433	0.47044	-0.03488
B	0.32912	0.63601	-0.00857
B	0.32857	0.13856	0.00111
B	0.65847	0.13858	0.00114
B	0.49388	0.30822	0.00602
B	0.33053	0.79904	0.01505
B	0.82351	0.30819	0.00598
B	0.16083	0.47042	-0.03486
B	0.66083	0.47042	-0.03486
B	0.16045	0.63601	-0.00854
B	0.99602	0.79903	0.01509
B	0.32351	0.30819	0.00598
B	0.16021	0.97079	0.02310
B	0.49433	0.47044	-0.03488
B	0.82912	0.63601	-0.00857
B	0.83053	0.79904	0.01505
B	0.66021	0.97079	0.02310
B	0.99459	0.97079	0.02313
B	0.82857	0.13856	0.00111
B	0.66045	0.63601	-0.00854
B	0.15847	0.13858	0.00114
B	0.49602	0.79903	0.01509
B	0.99388	0.30822	0.00602
B	0.32626	0.97308	0.00120
B	0.32902	0.46755	-0.04080
B	0.82626	0.97308	0.00120
B	0.65520	0.31519	0.02490
B	0.82902	0.46755	-0.04080
B	0.66081	0.80396	-0.00730
B	0.15520	0.31519	0.02490
B	0.16081	0.80396	-0.00730
Li	1.01968	0.58622	0.08438
Li	0.51968	0.58622	0.08438
Li	0.98477	0.15603	0.10775
Li	0.48477	0.15603	0.10775

Li_4/BBP under an applied electric field of 0.10 V Å^{-1}

B	0.49459	0.97080	0.02311
B	0.99433	0.47044	-0.03487
B	0.32912	0.63602	-0.00857
B	0.32857	0.13857	0.00113
B	0.65846	0.13859	0.00116
B	0.49388	0.30822	0.00605
B	0.33055	0.79903	0.01501
B	0.82352	0.30818	0.00600
B	0.16083	0.47043	-0.03485
B	0.66083	0.47043	-0.03485
B	0.16044	0.63601	-0.00855
B	0.99602	0.79902	0.01505
B	0.32352	0.30818	0.00600
B	0.16020	0.97080	0.02308
B	0.49433	0.47044	-0.03487
B	0.82912	0.63602	-0.00857
B	0.83055	0.79903	0.01501
B	0.66020	0.97080	0.02308
B	0.99459	0.97080	0.02311
B	0.82857	0.13857	0.00113
B	0.66044	0.63601	-0.00855
B	0.15846	0.13859	0.00116
B	0.49602	0.79902	0.01505
B	0.99388	0.30822	0.00605
B	0.32626	0.97309	0.00120
B	0.32902	0.46755	-0.04079
B	0.82626	0.97309	0.00120
B	0.65520	0.31519	0.02491
B	0.82902	0.46755	-0.04079
B	0.66081	0.80396	-0.00732
B	0.15520	0.31519	0.02491
B	0.16081	0.80396	-0.00732
Li	1.01966	0.58624	0.08439
Li	0.51966	0.58624	0.08439
Li	0.98479	0.15599	0.10777
Li	0.48479	0.15599	0.10777

Li_4/BBP under an applied electric field of 0.15 V Å^{-1}

B	0.49452	0.97106	0.02171
B	0.99431	0.47034	-0.03448
B	0.32923	0.63595	-0.00840
B	0.32850	0.13882	0.00125
B	0.65828	0.13882	0.00126
B	0.49382	0.30831	0.00691
B	0.33043	0.79925	0.01394
B	0.82348	0.30830	0.00688
B	0.16094	0.47034	-0.03445
B	0.66094	0.47034	-0.03445
B	0.16041	0.63594	-0.00839
B	0.99592	0.79925	0.01395
B	0.32348	0.30830	0.00688
B	0.16002	0.97106	0.02172
B	0.49431	0.47034	-0.03448
B	0.82923	0.63595	-0.00840
B	0.83043	0.79925	0.01394
B	0.66002	0.97106	0.02172
B	0.99452	0.97106	0.02171
B	0.82850	0.13882	0.00125
B	0.66041	0.63594	-0.00839
B	0.15828	0.13882	0.00126
B	0.49592	0.79925	0.01395
B	0.99382	0.30831	0.00691
B	0.32619	0.97321	0.00133
B	0.32915	0.46732	-0.04046
B	0.82619	0.97321	0.00133
B	0.65520	0.31519	0.02514
B	0.82915	0.46732	-0.04046
B	0.66084	0.80390	-0.00799
B	0.15520	0.31519	0.02514
B	0.16084	0.80390	-0.00799
Li	1.01929	0.58697	0.08520
Li	0.51929	0.58697	0.08520
Li	0.98573	0.15411	0.10879
Li	0.48573	0.15411	0.10879

Li_4/BBP under an applied electric field of 0.20 V $Å^{-1}$

B	0.49452	0.97117	0.02132
B	0.99423	0.47037	-0.03434
B	0.32926	0.63591	-0.00828
B	0.32853	0.13884	0.00128
B	0.65823	0.13885	0.00129
B	0.49373	0.30835	0.00717
B	0.33044	0.79929	0.01355
B	0.82354	0.30832	0.00714
B	0.16098	0.47037	-0.03431
B	0.66098	0.47037	-0.03431
B	0.16041	0.63591	-0.00827
B	0.99586	0.79929	0.01356
B	0.32354	0.30832	0.00714
B	0.15992	0.97116	0.02131
B	0.49423	0.47037	-0.03434
B	0.82926	0.63591	-0.00828
B	0.83044	0.79929	0.01355
B	0.65992	0.97116	0.02131
B	0.99452	0.97117	0.02132
B	0.82853	0.13884	0.00128
B	0.66041	0.63591	-0.00827
B	0.15823	0.13885	0.00129
B	0.49586	0.79929	0.01356
B	0.99373	0.30835	0.00717
B	0.32616	0.97327	0.00135
B	0.32919	0.46723	-0.04057
B	0.82616	0.97327	0.00135
B	0.65523	0.31513	0.02493
B	0.82919	0.46723	-0.04057
B	0.66086	0.80386	-0.00810
B	0.15523	0.31513	0.02493
B	0.16086	0.80386	-0.00810
Li	1.01916	0.58722	0.08557
Li	0.51916	0.58722	0.08557
Li	0.98599	0.15359	0.10931
Li	0.48599	0.15359	0.10931

Li_4/BBP under an applied electric field of 0.25 V $Å^{-1}$

B	0.49454	0.97125	0.02097
B	0.99415	0.47040	-0.03419
B	0.32928	0.63589	-0.00819
B	0.32854	0.13887	0.00132
B	0.65819	0.13888	0.00133
B	0.49365	0.30833	0.00743
B	0.33045	0.79934	0.01312
B	0.82365	0.30830	0.00740
B	0.16105	0.47039	-0.03417
B	0.66105	0.47039	-0.03417
B	0.16041	0.63589	-0.00817
B	0.99581	0.79934	0.01313
B	0.32365	0.30830	0.00740
B	0.15980	0.97125	0.02096
B	0.49415	0.47040	-0.03419
B	0.82928	0.63589	-0.00819
B	0.83045	0.79934	0.01312
B	0.65980	0.97125	0.02096
B	0.99454	0.97125	0.02097
B	0.82854	0.13887	0.00132
B	0.66041	0.63589	-0.00817
B	0.15819	0.13888	0.00133
B	0.49581	0.79934	0.01313
B	0.99365	0.30833	0.00743
B	0.32613	0.97334	0.00137
B	0.32925	0.46711	-0.04071
B	0.82613	0.97334	0.00137
B	0.65525	0.31509	0.02470
B	0.82925	0.46711	-0.04071
B	0.66087	0.80383	-0.00820
B	0.15525	0.31509	0.02470
B	0.16087	0.80383	-0.00820
Li	1.01901	0.58753	0.08594
Li	0.51901	0.58753	0.08594
Li	0.98624	0.15310	0.10987
Li	0.48624	0.15310	0.10987