Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Magnetic Couplings and Applied Electric Field Regulation in Diradical SiC Defect Diamond-like Nanoclusters

Xuexing Lin, Yuxiang Bu*

School of Chemistry and Chemical Engineering, Shandong University, Jinan, 250100, P. R. China

Electronic Supplementary Information

Table S1. The total energies of BS, T and CS states with their corresponding $\langle S^2 \rangle$, *J* and *d* values of the SiC clusters with different defect centers, calculated at the B3LYP/6-311++G(d, p) level.

Cluster	$E_{BS}(\langle S^2 \rangle)$ (a.u.)	$E_T(\langle S^2 \rangle)$ (a.u.)	E_{CS} (a.u.)	*J* (cm^{-1})	*d* (Å)
SiC-NVe	-5860.31875(1.009)	-5860.32308(2.021)	-5860.29042	938.5	3.793
SiC-NVeF	-9435.42725(1.014)	-9435.43347(2.023)	-9435.39923	1352.3	3.639
SiC-NVe-1	-10264.89955(1.009)	-10264.90562(2.018)	-10264.87231	1321.9	3.325
SiC-NVeF-1	-16220.91324(1.010)	-16220.91956(2.019)	-16220.88794	1376.1	3.405
SiC-NNV	-5876.97514(0.984)	-5876.97416(2.008)	-5876.96787	-211.4	3.908
SiC-NBV	-5846.94247(0.966)	-5846.94083(2.008)	-5846.93969	-344.7	3.827
SiC-BBV	-5816.90965(0.913)	-5816.90617(2.008)	-5816.91072	-	1.738
SiC-NNVF	-9451.96003(0.970)	-9451.95848(2.006)	-9451.94116	-329.3	3.754
SiC-NBVF	-9421.90454(0.940)	-9421.90197(2.007)	-9421.89826	-528.9	3.672
SiC-BBVF	-9391.84866(0.866)	-9391.84361(2.007)	-9391.84516	-972.1	3.559
SiC-NNV-1	-10281.57722(0.941)	-10281.57465(2.008)	-10281.55728	-528.7	3.401
SiC-NBV-1	-10251.54123(0.898)	-10251.53724(2.009)	-10251.52613	-787.5	3.418
SiC-BBV-1	-10221.50666(0.798)	-10221.49948(2.009)	-10221.49793	-1300.6	3.428

Table S2 The spacing *d* (Å) of any two atoms and corresponding total spin population (a.u.) in the defect center of the clusters with different defect centers, calculated at the B3LYP/6-311++G(d,p) level.

Cluster	**N···C_1**	**N···C_2**	**N···C_3**	**C_1···C_2**	**C_1···C_3**	**C_2···C_3**	**N**	**C_1**	**C_2**	**C_3**
SiC-NVe	3.844	3.841	3.841	3.796	3.796	3.793	0.024	0.740	0.738	0.738
SiC-NVeF	3.759	3.758	3.758	3.641	3.641	3.639	0.043	0.570	0.568	0.568
SiC-NVe-1	3.485	3.486	3.486	3.326	3.326	3.325	-0.043	0.616	0.616	0.616
SiC-NVeF-1	3.558	3.558	3.558	3.406	3.406	3.405	-0.038	0.595	0.595	0.595
Cluster	**N_1···N_2**	**N_1···C_2**	**N_1···C_3**	**N_2···C_2**	**N_2···C_3**	**C_2···C_3**	**N_1**	**N_2**	**C_2**	**C_3**
SiC-NNV	3.716	3.815	3.815	3.814	3.814	3.908	0.000	0.000	1.335	-1.335
SiC-NNVF	3.709	3.738	3.738	3.739	3.739	3.754	0.000	0.000	0.804	-0.804
SiC-NNV-1	3.507	3.471	3.471	3.472	3.472	3.401	0.000	0.000	0.582	-0.582
Cluster	**N···B**	**N···C_2**	**N···C_3**	**B···C_2**	**B···C_3**	**C_2···C_3**	**N**	**B**	**C_2**	**C_3**
SiC-NBV	3.905	4.006	4.006	3.748	3.748	3.827	0.000	0.000	1.085	-1.085
SiC-NBVF	3.796	3.692	3.692	3.823	3.823	3.672	0.000	0.000	0.786	-0.786
SiC-NBV-1	3.440	3.496	3.496	3.389	3.389	3.418	0.000	0.000	-0.765	0.765
Cluster	**B_1···B_2**	**B_1···C_2**	**B_1···C_3**	**B_2···C_2**	B_2···C_3	**C_2···C_3**	**B_1**	**B_2**	**C_2**	**C_3**
SiC-BBV	4.444	3.623	3.623	3.623	3.623	1.738	0.000	0.000	0.000	0.000
SiC-BBVF	3.943	3.750	3.750	3.751	3.751	3.559	0.000	0.000	0.804	-0.804
SiC-BBV-1	3.402	3.415	3.415	3.415	3.415	3.428	0.000	0.000	-0.796	0.796

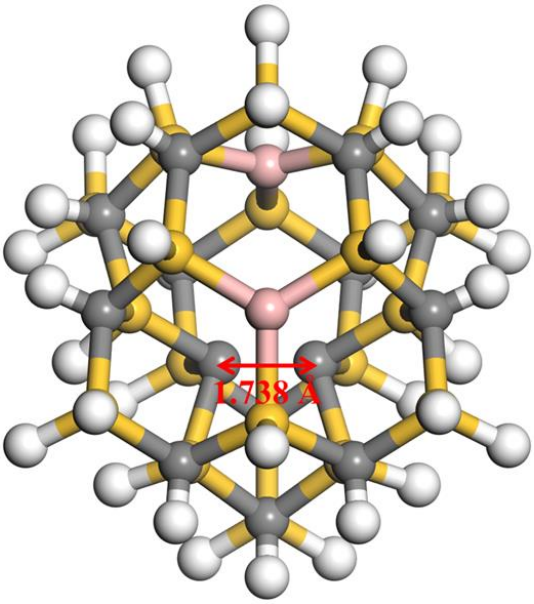

Figure S1. The SiC-BBV cluster featuring a long C-C single bond

Table S3. The orbital levels and their gaps between HOMO and LUMO (eV) of the clusters with different defect centers, calculated at the B3LYP/6-311++G(d, p) level.

Cluster	HOMO	LUMO	Gap
SiC-NVe	-2.204	-0.659	1.545
SiC-NVeF	-6.045	-4.159	1.886
SiC-NVe-1	-2.019	0.042	2.061
SiC-NVeF-1	-6.147	-4.293	1.854
SiC-NNV	-6.526	-3.450	3.077
SiC-NBV	-6.559	-3.614	2.946
SiC-BBV	-6.912	-3.311	3.601
SiC-NNVF	-9.792	-7.041	2.751
SiC-NBVF	-9.771	-7.289	2.482
SiC-BBVF	-9.655	-7.631	2.024
SiC-NNV-1	-5.668	-2.569	3.099
SiC-NBV-1	-5.761	-2.929	2.832
SiC-BBV-1	-6.020	-3.363	2.657

Table S4. The electronic configuration of doping N and B atoms and C-radicals in the defect center of the clusters with different defect centers through the NBO analysis, calculate at the B3LYP/6-311++G(d, p) level.

Cluster	N or B	C_1, N or B	C_2	C_3
SiC-NVe	N, 2s(0.76)2p(2.60)	C_1, 2s(0.65)2p(1.81)	α, 2s(0.65)2p(1.81)	α, 2s(0.65)2p(1.81)
SiC-NVeF	N, 2s(0.78)2p(2.61)	C_1, 2s(0.68)2p(1.80)	α, 2s(0.68)2p(1.80)	α, 2s(0.68)2p(1.80)
SiC-NVe-1	N, 2s(0.78)2p(2.69)	C_1, 2s(0.65)2p(1.83)	α, 2s(0.65)2p(1.83)	α, 2s(0.65)2p(1.83)
SiC-NVeF-1	N, 2s(0.78)2p(2.67)	C_1, 2s(0.65)2p(1.85)	α, 2s(0.65)2p(1.85)	α, 2s(0.65)2p(1.85)
SiC-NNV	N, 2s(0.76)2p(2.60)	N, 2s(0.76)2p(2.60)	α, 2s(0.66)2p(1.55)	β, 2s(0.69)2p(2.38)
SiC-NBV	N, 2s(0.77)2p(2.59)	B, 2s(0.56)2p(1.01)	β, 2s(0.69)2p(2.36)	α, 2s(0.66)2p(1.55)
SiC-BBV	B, 2s(0.56)2p(0.98)	B, 2s(0.56)2p(0.98)	-, 2s(0.61)2p(2.09)	-, 2s(0.61)2p(2.09)
SiC-NNVF	N, 2s(0.78)2p(2.61)	N, 2s(0.78)2p(2.61)	β, 2s(0.72)2p(2.40)	α, 2s(0.69)2p(1.55)
SiC-NBVF	N, 2s(0.78)2p(2.60)	B, 2s(0.60)2p(1.14)	β, 2s(0.72)2p(2.39)	α, 2s(0.69)2p(1.56)
SiC-BBVF	B, 2s(0.60)2p(1.13)	B, 2s(0.60)2p(1.14)	β, 2s(0.73)2p(2.35)	α, 2s(0.70)2p(1.57)
SiC-NNV-1	N, 2s(0.78)2p(2.67)	N, 2s(0.78)2p(2.67)	α, 2s(0.66)2p(1.47)	β, 2s(0.70)2p(2.20)
SiC-NBV-1	N, 2s(0.78)2p(2.67)	B, 2s(0.53)2p(0.65)	β, 2s(0.69)2p(2.17)	α, 2s(0.66)2p(1.46)
SiC-BBV-1	B, 2s(0.51)2p(0.81)	B, 2s(0.51)2p(0.81)	β, 2s(0.67)2p(1.88)	α, 2s(0.67)2p(1.88)

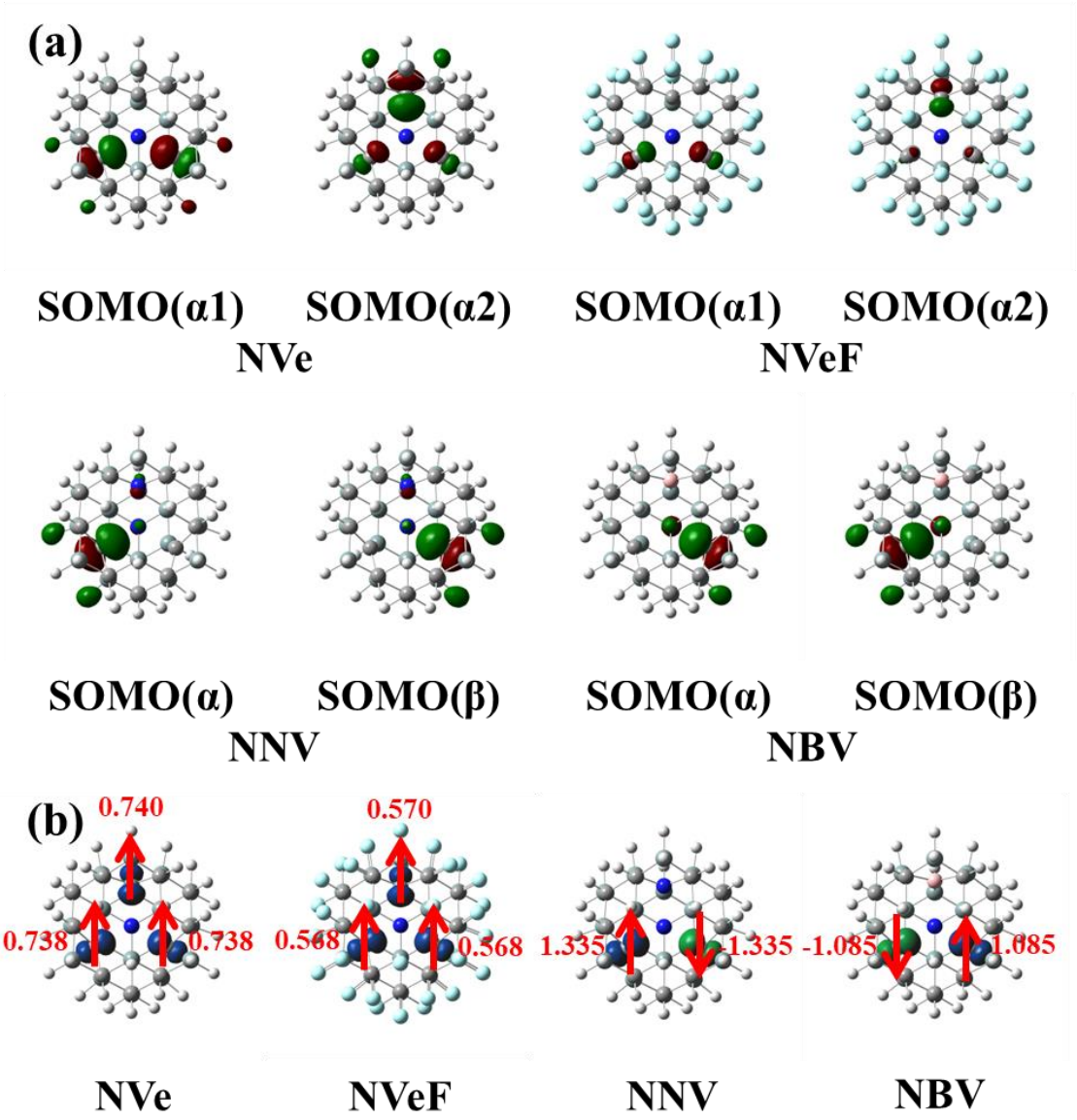

Figure S2. The (**a)** singly occupied molecular orbital (isovalue = 0.05) and (**b**) spin density distribution (isovalue = 0.01) of the clusters with different defect centers, calculated at the B3LYP/6-311++G(d, p) level.

Table S5. The total energy, *J* and *d* of the SiC-NVe cluster under an applied electric field (Intensity, *I*) (a.u.), calculated at the B3LYP/6-311++G(d, p) level.

Cluster	***I***	**E_{BS}(<S^2>) (a.u.)**	**E_T(<S^2>) (a.u.)**	**E_{CS} (a.u.)**	***J*** **(cm^{-1})**	***d*** **(Å)**
SiC-NVe	-0.012	-5860.38674(0.991)	-5860.38627(2.009)	-5860.38246	-102.0	3.880
(y-axis)	-0.010	-5860.36801(0.993)	-5860.36776(2.009)	-5860.36283	-54.8	3.887
	-0.008	-5860.35230(0.997)	-5860.35233(2.010)	-5860.34616	8.1	3.909
	-0.006	-5860.33957(1.000)	-5860.33997(2.011)	-5860.33235	87.3	3.899
	-0.004	-5860.32970(1.003)	-5860.33077(2.014)	-5860.32136	231.4	3.881
	-0.002	-5860.32275(1.007)	-5860.32499(2.019)	-5860.29290	485.5	3.840
	0.000	-5860.31875(1.009)	-5860.32308(2.021)	-5860.29042	938.5	3.793
	0.002	-5860.31775(1.008)	-5860.32479(2.021)	-5860.29157	1526.1	3.778
	0.004	-5860.31983(1.002)	-5860.32967(2.020)	-5860.29907	2121.4	3.777
	0.006	-5860.32508(0.987)	-5860.33752(2.019)	-5860.30799	2645.1	3.782
	0.008	-5860.33360(0.959)	-5860.34828(2.019)	-5860.32002	3038.3	3.791
	0.010	-5860.34545(0.912)	-5860.36194(2.020)	-5860.33522	3266.2	3.802
	0.012	-	-	-	-	-
SiC-NVe	-0.012	-	-	-	-	-
(z-axis)	-0.010	-	-	-	-	-
	-0.008	-5860.34562(1.009)	-5860.34978(2.024)	-5860.31705	899.6	3.820
	-0.006	-5860.33479(1.009)	-5860.33900(2.023)	-5860.30626	911.8	3.812
	-0.004	-5860.32671(1.009)	-5860.33097(2.022)	-5860.29824	922.2	3.806
	-0.002	-5860.32137(1.009)	-5860.32566(2.022)	-5860.29296	931.0	3.799
	0.000	-5860.31875(1.009)	-5860.32308(2.021)	-5860.29042	938.5	3.793
	0.002	-5860.31886(1.009)	-5860.32321(2.021)	-5860.29060	944.7	3.788
	0.004	-5860.32169(1.009)	-5860.32607(2.021)	-5860.29353	949.7	3.782
	0.006	-5860.32727(1.009)	-5860.33167(2.021)	-5860.29921	953.6	3.777
	0.008	-5860.33562(1.009)	-5860.34003(2.022)	-5860.30766	956.5	3.772
	0.010	-5860.34677(1.009)	-5860.35119(2.022)	-5860.31893	958.4	3.768
	0.012	-5860.36078(1.009)	-5860.36521(2.022)	-5860.33307	959.5	3.763

Table S6. The spacing *d* (Å) of any two atoms and corresponding total spin population (a.u.) in the defect center of the SiC-NVe cluster under an applied electric field (a.u.), calculated at the B3LYP/6-311++G(d, p) level.

Cluster	***I***	**N···C$_1$**	**N···C$_2$**	**N···C$_3$**	**C$_1$···C$_2$**	**C$_1$···C$_3$**	**C$_2$···C$_3$**	**N**	**C$_1$**	**C$_2$**	**C$_3$**
SiC-NVe	-0.012	3.906	3.832	3.832	3.972	3.972	3.880	0.000	0.000	-1.169	1.169
(y-axis)	-0.010	3.888	3.837	3.837	3.948	3.948	3.887	0.000	0.000	-1.149	1.149
	-0.008	3.856	3.849	3.849	3.901	3.901	3.909	0.012	0.034	1.199	1.199
	-0.006	3.839	3.852	3.852	3.865	3.865	3.899	0.014	0.085	1.146	1.146
	-0.004	3.826	3.853	3.853	3.829	3.829	3.881	0.018	0.189	1.063	1.063
	-0.002	3.826	3.850	3.850	3.796	3.796	3.840	0.022	0.415	0.916	0.916
	0.000	3.844	3.841	3.841	3.796	3.796	3.793	0.024	0.740	0.738	0.738
	0.002	3.854	3.837	3.837	3.813	3.813	3.778	0.023	0.935	0.647	0.647
	0.004	3.859	3.837	3.837	3.830	3.830	3.777	0.022	1.049	0.598	0.598
	0.006	3.860	3.839	3.839	3.845	3.845	3.782	0.020	1.124	0.570	0.570
	0.008	3.859	3.843	3.843	3.860	3.860	3.791	0.018	1.181	0.552	0.552
	0.010	3.857	3.847	3.847	3.874	3.874	3.802	0.017	1.228	0.544	0.544
	0.012	-	-	-	-	-	-	-	-	-	-
SiC-NVe	-0.012	-	-	-	-	-	-	-	-	-	-
(z-axis)	-0.010	-	-	-	-	-	-	-	-	-	-
	-0.008	3.833	3.831	3.831	3.822	3.822	3.820	0.021	0.721	0.719	0.719
	-0.006	3.835	3.832	3.832	3.815	3.815	3.812	0.021	0.727	0.725	0.725
	-0.004	3.837	3.835	3.835	3.808	3.808	3.806	0.022	0.732	0.730	0.730
	-0.002	3.840	3.838	3.838	3.802	3.802	3.799	0.023	0.737	0.735	0.735
	0.000	3.844	3.841	3.841	3.796	3.796	3.793	0.024	0.740	0.738	0.738
	0.002	3.848	3.845	3.845	3.790	3.790	3.788	0.026	0.744	0.742	0.742
	0.004	3.853	3.850	3.850	3.785	3.785	3.782	0.027	0.747	0.745	0.745
	0.006	3.858	3.855	3.855	3.780	3.780	3.777	0.028	0.750	0.748	0.748
	0.008	3.864	3.861	3.861	3.775	3.775	3.772	0.028	0.753	0.751	0.751
	0.010	3.870	3.867	3.867	3.770	3.770	3.768	0.025	0.756	0.756	0.756
	0.012	3.877	3.874	3.874	3.765	3.765	3.763	0.014	0.766	0.764	0.764

Table S7. The orbital levels and their gaps between HOMO and LUMO (eV) of the SiC-NVe cluster under an applied electric field in y and z-axes (a.u.), calculated at the B3LYP/6-311++G(d, p) level.

I	**Cluster**	**HOMO**	**LUMO**	**Gap**	**Cluster**	**HOMO**	**LUMO**	**Gap**
-0.012	SiC-NVe	-2.750	-1.005	1.746	SiC-NVe	-	-	-
-0.010	(y-axis)	-2.626	-0.558	2.069	(z-axis)	-	-	-
-0.008		-2.527	-0.753	1.774		-2.353	-0.841	1.512
-0.006		-2.421	-0.759	1.662		-2.310	-0.787	1.522
-0.004		-2.323	-0.761	1.562		-2.271	-0.739	1.531
-0.002		-2.238	-0.739	1.499		-2.235	-0.697	1.539
0.000		-2.204	-0.659	1.545		-2.204	-0.659	1.545
0.002		-2.220	-0.742	1.478		-2.176	-0.625	1.551
0.004		-2.255	-0.818	1.437		-2.151	-0.595	1.556
0.006		-2.298	-0.892	1.407		-2.130	-0.569	1.562
0.008		-2.350	-0.968	1.381		-2.114	-0.547	1.566
0.010		-2.409	-1.051	1.358		-2.101	-0.531	1.570
0.012		-	-	-		-2.094	-0.827	1.267

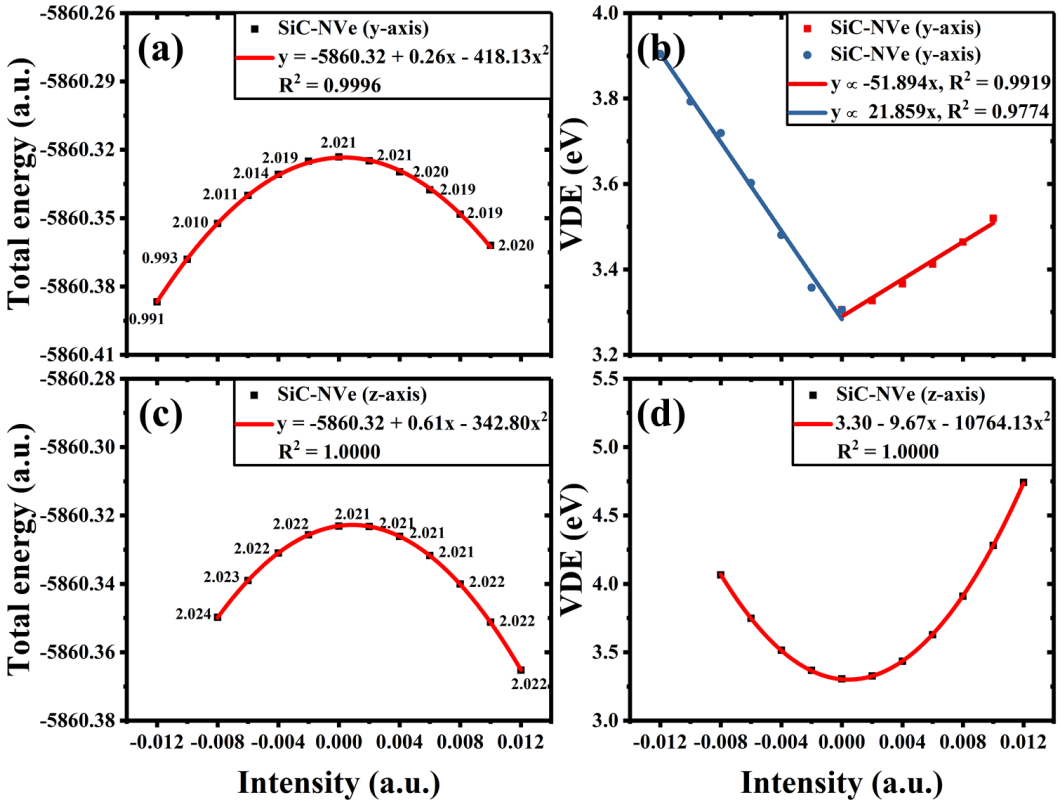

Figure S3. The total energy and the corresponding VDE of the SiC-NVe cluster under an applied electric field in (**a**) and (**b**) y-axis and (**c**) and (**d**) z-axis respectively，calculated at the B3LYP/6-311++G(d, p) level.

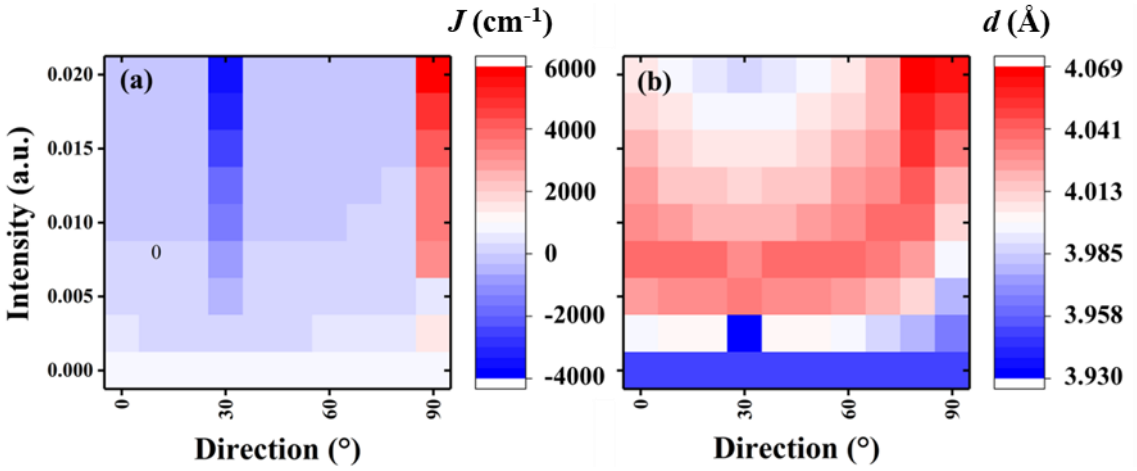

Figure S4. The (**a**) *J* and (**b**) *d* of SiC-NVe cluster under an applied electric field at each angular direction of the C-radical plane, calculated at the B3LYP/6-311G(d, p) level.

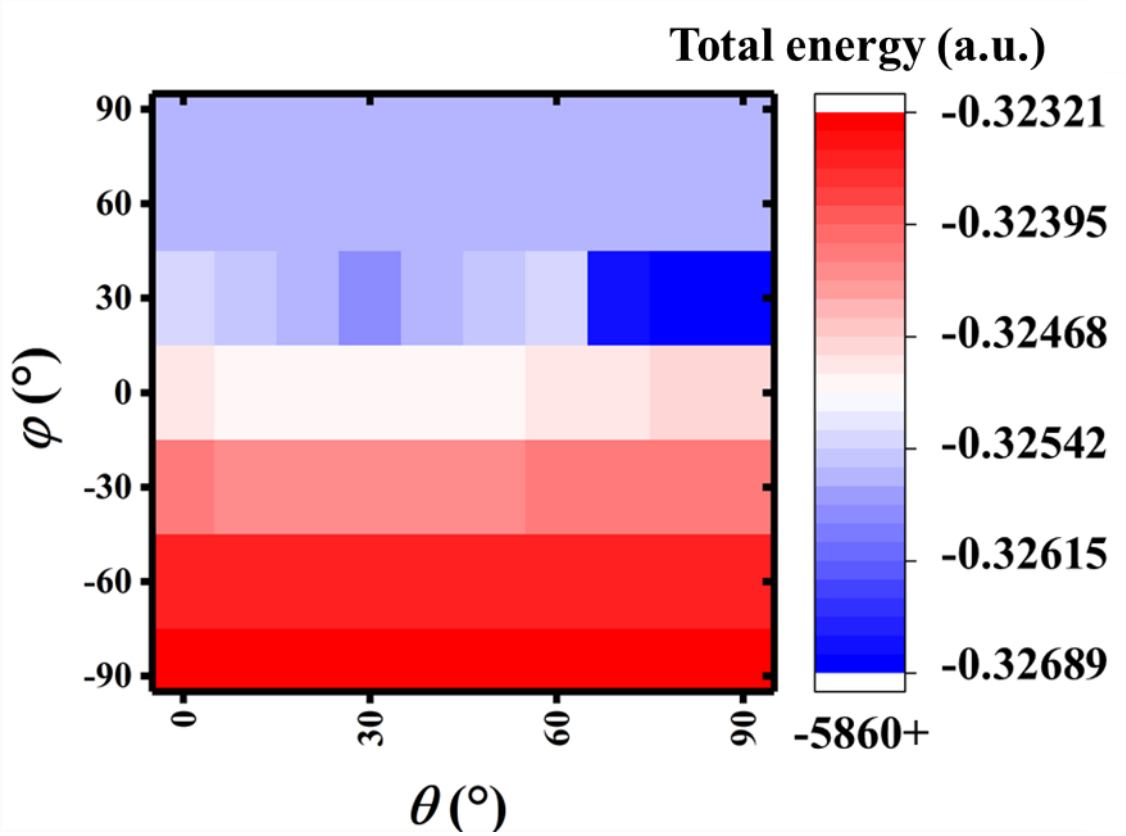

Figure S5. The total energy (a.u.) of the SiC-NVe cluster (taking $|I|$ = 0.002 a.u. as an example) under an applied electric field at each angle (θ, φ) in space, calculated at the B3LYP/6-311++G(d, p) level.

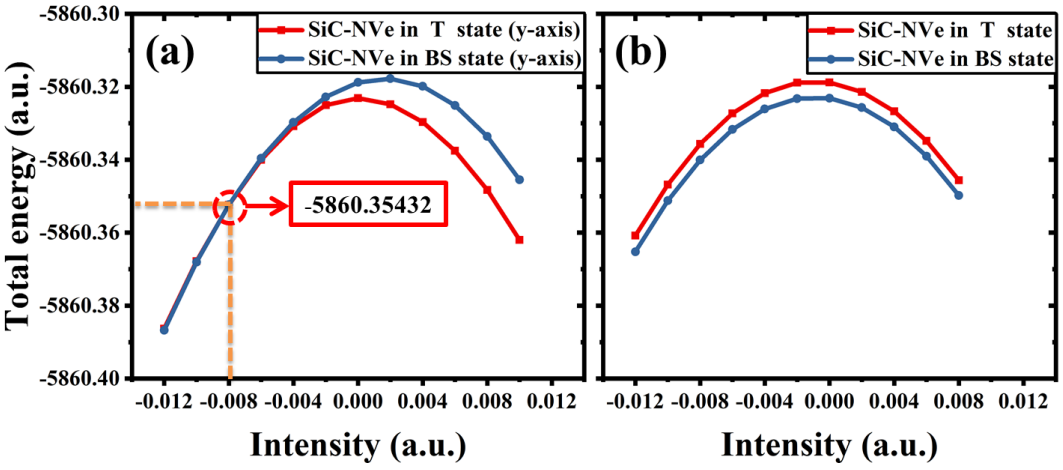

Figure S6. The total energy (a.u.) in (**a**) y-axis and (**b**) z-axis of the SiC-NVe cluster under an applied electric field respectively, calculated at the B3LYP/6-311++G(d, p) level.

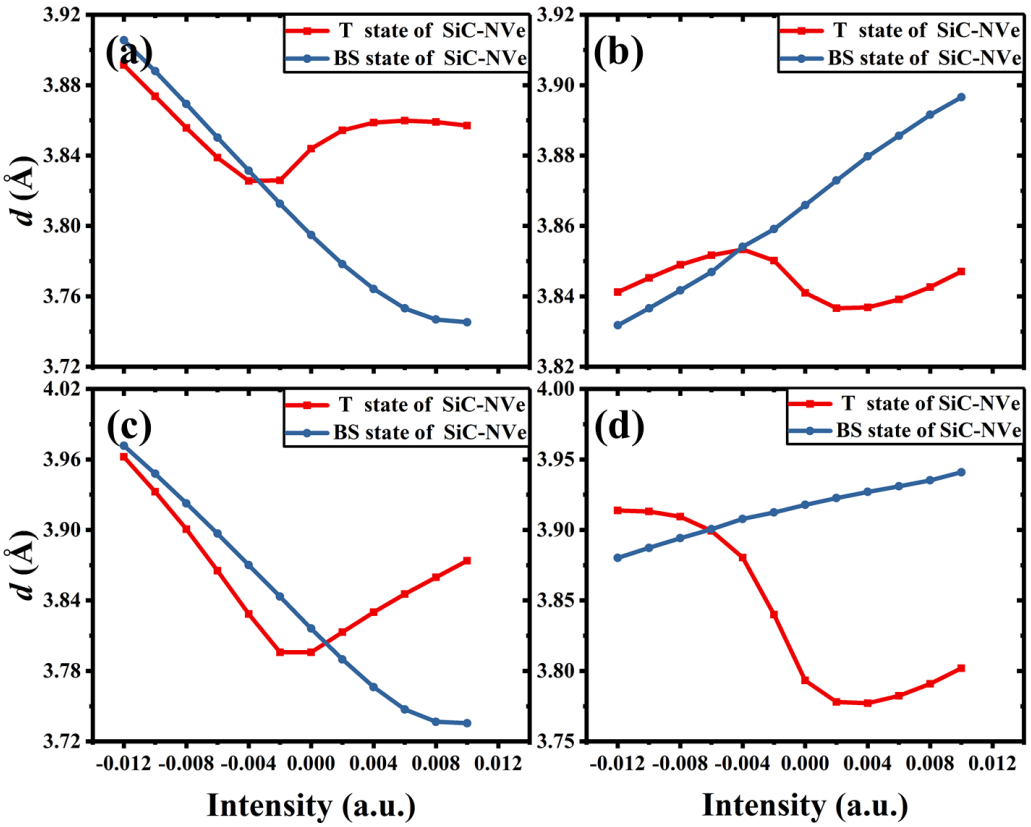

Figure S7. The relationships between the electric field intensity and the spacing *d* (**a**) N...C_1, (**b**) N...C_2 (C_3), (**c**) C_1...C_2 (C_3) and (**d**) C_2...C_3 of any two atoms in the defect center of the SiC-NVe cluster in the T and BS states, respectively, under an applied electric field in y-axis, calculated at the B3LYP/6-311++G(d, p) level.

Table S8. The energy levels (a.u.) and the two average energy levels (eV) of SOMO(α1), SOMO(α2), SOMO(α3) and SOMO(β1) (or HOMO) in the T state or SOMO(α), SOMO(β), NSOMO(α) and NSOMO(β) in the BS state of the SiC-NVe cluster under an applied electric field (Intensity, *I*) (a.u.), calculated at the B3LYP/6-311++G(d, p) level.

I	**SOMO(α1) or SOMO(α)**	**SOMO(α2) or SOMO(β)**	**SOMO(α3) or NSOMO(α)**	**SOMO(β1) or NSOMO(β)**	**Average-1**	**Average-2**
-0.012	-0.10107	-0.10107	-0.13547	-0.13547	-2.750	-3.218
-0.010	-0.09651	-0.09651	-0.13570	-0.13570	-2.626	-3.159
-0.008	-0.09691	-0.12736	-0.14036	-0.09287	-3.051	-3.112
-0.006	-0.09615	-0.12679	-0.13995	-0.08897	-3.033	-3.074
-0.004	-0.09808	-0.12501	-0.13887	-0.08537	-3.035	-3.043
-0.002	-0.10531	-0.12028	-0.13636	-0.08223	-3.069	-3.022
0.000	-0.11374	-0.11383	-0.13456	-0.08099	-3.096	-3.014
0.002	-0.11118	-0.11606	-0.13498	-0.08160	-3.092	-3.019
0.004	-0.11088	-0.11670	-0.13515	-0.08286	-3.096	-3.031
0.006	-0.11167	-0.11696	-0.13507	-0.08446	-3.111	-3.049
0.008	-0.11314	-0.11697	-0.13510	-0.08635	-3.131	-3.072
0.010	-0.11516	-0.11672	-0.13556	-0.08853	-3.155	-3.102
0.012	-	-	-	-	-	-

Note: Average-1 is the average of first two SOMOs in the Table, while Average-2 is all.

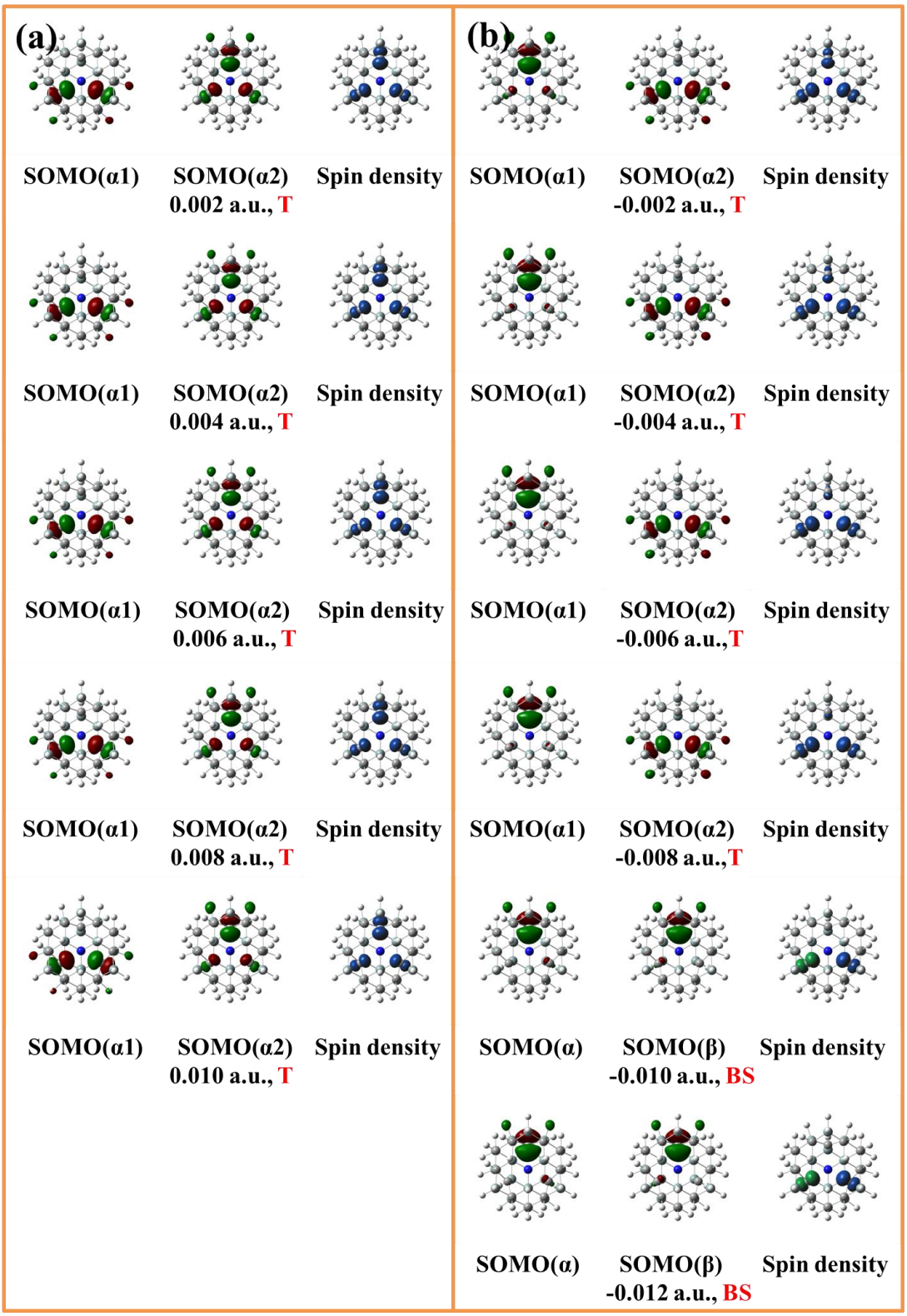

Figure S8. The singly occupied molecular orbital (isovalue = 0.05) and the spin density distribution (isovalue = 0.01) of the SiC-NVe cluster under (**a**) an applied positive and (**b**) an applied negative electric field in y-axis, calculated at the B3LYP/6-311++G(d, p) level.