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NFeN 结构和性质及反应势能曲线

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Structures and Properties of NFeN and the Reaction Potential Energy Curves

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附表 S1　五重态 B-NFeN 的电子结构参数

Table S1　Partial molecular orbitals occupation, natural electronic configuration, natural and Mulliken charges, and total spin densities (TSD) for B-NFeN(2*S*+1=5) molecule

State	Molecular orbital occupation	Natural electronic configuration	Natural charge(*e*)	Mulliken charge(*e*)	TSD(*e*)
1^5A_1	α: $5b_2 3b_1 9a_1 6b_2 4b_1 10a_1 2a_2$	$4s^{0.09}3d^{6.84}4p^{0.07}$(Fe)	0.774	0.328	1.511
	β: $1a_2 9a_1 3b_1$	$2s^{1.93}2p^{3.58}$(N)	-0.387	-0.164	1.244
2^5A_1	α: $1a_2 3b_1 9a_1 4b_1 10a_1 6b_2 11a_1$	$4s^{0.41}3d^{6.75}4p^{0.03}$	0.814	0.306	1.216
	β: $8a_1 9a_1 6b_2$	$2s^{1.93}2p^{3.47}$	-0.407	-0.153	1.392
3^5A_1	α: $1a_2 5b_2 9a_1 10a_1 6b_2 11a_1 7b_2$	$4s^{0.43}3d^{6.48}4p^{0.04}$	1.044	0.352	3.614
	β: $3b_1 5b_2 9a_1$	$2s^{1.95}2p^{3.57}$	-0.522	-0.176	0.193
4^5A_1	α: $1a_2 9a_1 3b_1 6b_2 10a_1 11a_1 4b_1$	$4s^{0.35}3d^{6.65}4p^{0.05}$	0.962	0.338	2.296
	β: $3b_1 9a_1 4b_1$	$2s^{1.91}2p^{3.57}$	-0.481	-0.169	0.852
1^5B_1	α: $1a_2 9a_1 3b_1 10a_1 4b_1 6b_2 11a_1$	$4s^{0.42}3d^{6.75}4p^{0.03}$	0.800	0.272	1.004
	β: $8a_1 3b_1 6b_2$	$2s^{1.93}2p^{3.47}$	-0.400	-0.136	1.498
2^5B_1	α: $1a_2 3b_1 9a_1 6b_2 10a_1 4b_1 7b_2$	$4s^{0.29}3d^{6.86}4p^{0.03}$	0.822	0.332	0.302
	β: $5b_2 3b_1 9a_1$	$2s^{1.96}2p^{3.46}$	-0.411	-0.166	1.849
3^5B_1	α: $3b_1 1a_2 9a_1 6b_2 10a_1 11a_1 4b_1$	$4s^{0.44}3d^{6.72}4p^{0.04}$	0.816	0.332	1.938
	β: $9a_1 3b_1 10a_1$	$2s^{1.89}2p^{3.51}$	-0.408	-0.166	1.031
1^5A_2	α: $5b_2 9a_1 1a_2 6b_2 10a_1 4b_1 11a_1$	$4s^{0.383}d^{6.79}4p^{0.04}$	0.806	0.340	2.178
	β: $8a_1 9a_1 3b_1$	$2s^{1.91}2p^{3.48}$	-0.403	-0.170	0.910
1^5B_2	α: $3b_1 9a_1 1a_2 10a_1 6b_2 11a_1 4b_1$	$4s^{0.33}3d^{6.58}4p^{0.06}$	1.046	0.340	2.674
	β: $3b_1 9a_1 2a_2$	$2s^{1.91}2p^{3.60}$	-0.523	-0.170	0.666
2^5B_2	α: $9a_1 3b_1 10a_1 6b_2 11a_1 4b_1 7b_2$	$4s^{0.33}3d^{6.56}4p^{0.06}$	1.052	0.314	1.634
	β: $8a_1 3b_1 9a_1$	$2s^{1.97}2p^{3.56}$	-0.526	-0.157	1.183

附表 S2　三重态 B-NFeN 的电子结构参数

Table S2　Partial molecular orbitals occupation, natural electronic configuration, natural and Mulliken charges, and total spin densities (TSD) for B-NFeN(2*S*+1=3) molecule

State	Molecular orbital occupation	Natural electronic configuration	Natural charge(*e*)	Mulliken charge(*e*)	TSD(*e*)
1^3A_1	α: $8a_1 1a_2 5b_2 9a_1 3b_1 6b_2 10a_1 2a_2$	$4s^{0.17}3d^{6.85}4p^{0.06}$	0.948	0.406	-0.540
	β: $8a_1 3b_1 5b_2 1a_2 9a_1 4b_1$	$2s^{1.93}2p^{3.53}$	-0.474	-0.203	1.270
2^3A_1	α: $8a_1 5b_2 1a_2 9a_1 3b_1 10a_1 4b_1 6b_2$	$4s^{0.09}3d^{6.83}4p^{0.08}$	1.032	0.512	1.018
	β: $8a_1 1a_2 5b_2 3b_1 4b_1 6b_2$	$2s^{1.94}2p^{3.57}$	-0.516	-0.256	0.491
3^3A_1	α: $8a_1 1a_2 5b_2 9a_1 3b_1 10a_1 4b_1 11a_1$	$4s^{0.40}3d^{6.83}4p^{0.04}$	0.752	0.182	2.442
	β: $8a_1 5b_2 1a_2 3b_1 9a_1 4b_1$	$2s^{1.90}2p^{3.47}$	-0.376	-0.091	-0.221
4^3A_1	α: $8a_1 1a_2 5b_2 9a_1 3b_1 6b_2 10a_1 11a_1$	$4s^{0.25}3d^{6.77}4p^{0.06}$	0.944	0.440	0.724
	β: $3b_1 5b_2 8a_1 1a_2 9a_1 4b_1$	$2s^{1.92}2p^{3.54}$	-0.472	-0.220	0.638
5^3A_1	α: $8a_1 5b_2 9a_1 1a_2 6b_2 10a_1 11a_1 7b_2$	$4s^{0.44}3d^{6.56}4p^{0.04}$	0.968	0.318	1.400
	β: $3b_1 1a_2 8a_1 5b_2 4b_1 9a_1$	$2s^{1.93}2p^{3.55}$	-0.484	-0.159	0.300
6^3A_1	α: $8a_1 9a_1 1a_2 10a_1 3b_1 11a_1 5b_2 6b_2$	$4s^{0.78}3d^{6.09}4p^{0.08}$	1.058	0.058	0.798
	β: $8a_1 1a_2 9a_1 3b_1 10a_1 11a_1$	$2s^{1.92}2p^{3.61}$	-0.529	-0.029	0.601
1^3B_1	α: $8a_1 5b_2 3b_1 1a_2 9a_1 10a_1 4b_1 6b_2$	$4s^{0.25}3d^{6.89}4p^{0.06}$	0.824	0.370	1.834
	β: $8a_1 5b_2 1a_2 3b_1 9a_1 6b_2$	$2s^{1.92}2p^{3.48}$	-0.412	-0.185	0.083
2^3B_1	α: $8a_1 5b_2 1a_2 9a_1 6b_2 3b_1 10a_1 7b_2$	$4s^{0.17}3d^{6.85}4p^{0.06}$	1.006	0.390	-1.690
	β: $1a_2 8a_1 3b_1 5b_2 9a_1 4b_1$	$2s^{1.93}2p^{3.53}$	-0.503	-0.195	1.845
3^3B_1	α: $8a_1 9a_1 5b_2 3b_1 10a_1 6b_2 11a_1 4b_1$	$4s^{0.27}3d^{6.66}4p^{0.06}$	1.018	0.314	0.656
	β: $1a_2 3b_1 5b_2 8a_1 9a_1 4b_1$	$2s^{1.94}2p^{3.56}$	-0.509	-0.157	0.672
4^3B_1	α: $8a_1 1a_2 9a_1 5b_2 6b_2 10a_1 11a_1 2a_2$	$4s^{0.42}3d^{6.59}4p^{0.04}$	0.965	0.368	0.642
	β: $3b_1 5b_2 8a_1 1a_2 9a_1 4b_1$	$2s^{1.94}2p^{3.54}$	-0.482	-0.184	0.679
5^3B_1	α: $8a_1 5b_2 9a_1 1a_2 3b_1 10a_1 11a_1 4b_1$	$4s^{0.38}3d^{6.56}4p^{0.05}$	1.020	0.186	2.326
	β: $1a_2 8a_1 3b_1 4b_1 9a_1 2a_2$	$2s^{1.93}2p^{3.57}$	-0.510	-0.093	-0.163
1^3A_2	α: $8a_1 5b_2 9a_1 1a_2 3b_1 6b_2 10a_1 11a_1$	$4s^{0.38}3d^{6.84}4p^{0.04}$	0.762	0.342	0.998
	β: $3b_1 5b_2 1a_2 8a_1 9a_1 4b_1$	$2s^{1.91}2p^{3.46}$	-0.381	-0.171	0.501
1^3B_2	α: $8a_1 5b_2 1a_2 9a_1 3b_1 6b_2 10a_1 4b_1$	$4s^{0.20}3d^{6.96}4p^{0.05}$	0.810	0.400	0.628
	β: $8a_1 5b_2 1a_2 3b_1 9a_1 4b_1$	$2s^{1.92}2p^{3.48}$	-0.405	-0.200	0.686
2^3B_2	α: $8a_1 3b_1 5b_2 9a_1 1a_2 10a_1 11a_1 4b_1$	$4s^{0.42}3d^{6.41}4p^{0.07}$	1.122	0.140	3.374
	β: $1a_2 8a_1 5b_2 3b_1 9a_1 2a_2$	$2s^{1.92}2p^{3.63}$	-0.561	-0.070	-0.687
3^3B_2	α: $8a_1 5b_2 9a_1 3b_1 6b_2 10a_1 11a_1 7b_2$	$4s^{0.46}3d^{6.52}4p^{0.03}$	0.989	0.358	1.460
	β: $1a_2 8a_1 3b_1 5b_2 4b_1 9a_1$	$2s^{1.96}2p^{3.54}$	-0.494	-0.179	0.270
4^3B_2	α: $8a_1 5b_2 1a_2 9a_1 3b_1 10a_1 4b_1 11a_1$	$4s^{0.69}3d^{6.56}4p^{0.05}$	0.710	0.074	1.968
	β: $8a_1 1a_2 3b_1 4b_1 9a_1 10a_1$	$2s^{1.91}2p^{3.44}$	-0.355	-0.037	0.016

附表 S3　单重态 B-NFeN 的电子结构参数

Table S3　Partial molecular orbitals occupation, natural electronic configuration, natural and Mulliken charges, and total spin densities (TSD) for B-NFeN(2*S*+1=1) molecule

State	Molecular orbital occupation	Natural electronic configuration	Natural charge(*e*)	Mulliken charge(*e*)	TSD(*e*)
1^1A_1	α: $8a_1 5b_2 1a_2 9a_1 3b_1 10a_1 6b_2$	$4s^{0.36}3d^{7.09}4p^{0.02}$	0.542	0.316	0.0
	β: $8a_1 5b_2 1a_2 9a_1 3b_1 10a_1 6b_2$	$2s^{1.91}2p^{3.35}$	-0.271	-0.158	0.0
2^1A_1	α: $8a_1 5b_2 1a_2 3b_1 9a_1 6b_2 4b_1$	$4s^{0.08}3d^{6.95}4p^{0.07}$	0.924	0.502	0.0
	β: $8a_1 5b_2 1a_2 3b_1 9a_1 6b_2 4b_1$	$2s^{1.92}2p^{3.53}$	-0.462	-0.251	0.0
3^1A_1	α: $8a_1 5b_2 1a_2 9a_1 3b_1 4b_1 10a_1$	$4s^{0.08}3d^{7.33}4p^{0.04}$	0.600	0.400	0.0
	β: $8a_1 5b_2 1a_2 9a_1 3b_1 4b_1 10a_1$	$2s^{1.92}2p^{3.38}$	-0.300	-0.200	0.0
1^1B_1	α: $5b_2 1a_2 8a_1 3b_1 9a_1 4b_1 10a_1$	$4s^{0.42}3d^{6.88}4p^{0.05}$	0.688	0.228	0.404
	β: $8a_1 5b_2 1a_2 9a_1 3b_1 10a_1 11a_1$	$2s^{1.90}2p^{3.44}$	-0.344	-0.114	-0.202

表 S4　$D_{\infty h}$ 点群下碎片轨道对称变换性质

Table S4　Symmetry Transformation properties for orbital of $D_{\infty h}$ point group

$D_{\infty v}$	Fe	N
Σ_g^+	s, d_z^2	s
Π_g	(d_{xz}, d_{yz})	
Δ_g	(d_x^2-y^2, d_{xy})	
Σ_u^+	p_z	p_z
Π_u	(p_x, p_y)	(p_x, p_y)

附表 S5　Fe 原子插入 N_2 的过渡态 TS 的电子结构参数

Table S5　Partial molecular orbitals occupation, natural electronic configuration, natural and Mulliken charges(e), and total spin densities (TSD) for TS-FeN_2

State	Molecular orbital occupation	Natural electronic configuration	Natural charge(e)	Mulliken charge(e)	TSD
$^1A_1$	α: $5b_21a_29a_13b_14b_110a_1$	$4s^{0.18}3d^{7.23}4p^{0.03}$	0.576	0.378	0.0
	β: $5b_21a_29a_13b_14b_110a_1$	$2s^{1.91}2p^{3.36}$	-0.288	-0.189	0.0
1^3B_1	α: $5b_21a_23b_19a_110a_14b_111a_1$	$4s^{0.18}3d^{7.23}4p^{0.03}$	0.748	0.266	2.280
	β: $5b_21a_29a_13b_110a_1$	$2s^{1.91}2p^{3.36}$	-0.374	-0.133	-0.140
2^3B_1	α: $5b_21a_23b_19a_110a_14b_111a_1$	$4s^{0.23}3d^{6.56}4p^{0.09}$	1.102	0.362	2.400
	β: $5b_21a_29a_13b_110a_1$	$2s^{1.87}2p^{3.63}$	-0.551	-0.181	-0.200
1^5B_1	α: $5b_23b_19a_11a_210a_111a_16b_24b_1$	$4s^{0.44}3d^{6.67}4p^{0.04}$	0.860	0.300	2.560
	β: $3b_19a_11a_210a_1$	$2s^{1.89}2p^{3.53}$	-0.430	-0.150	0.720