《稀土掺杂硼团簇 REB_n^- (RE = La, Sc; n = 6, 8) 的几何及电子结构*》的补充材料

陈子俊 [1)] 李慧芳 [1)†] 谢圳明 [1)] 张勇航 [2)] 郑浩 [2)] 姜凯乐 [2)] 张博 [2)]

张家铭 [2)] 王怀谦 [1)2)‡]

1)（华侨大学工学院，泉州 362021）

2)（华侨大学信息科学与工程学院，厦门 361021）

补充材料 A: REB_n^- (RE = La, Sc; n = 6, 8)低能异构体的笛卡尔坐标

Suppl. A: Cartesian coordinates of the low−lying isomers of the REB_n^- (RE = La, Sc; n = 6, 8) clusters

表 S1 PBE1PBE/La/SDD/B/6−311+G*计算水平下，LaB_6^-低能异构体的笛卡尔坐标

Table S1. Cartesian coordinates of the low-lying isomers of the LaB_6^- clusters at the PBE1PBE/La/SDD/B/6−311+G* level.

Cluster	Atoms	*X*	*Y*	*Z*
LaB_6^--Ⅰ	B	−1.79113700	0.48102800	0.74105200
	B	−0.82430700	1.80550800	0.30725200
	B	−1.68074300	1.11063700	−0.82050800
	B	−1.68010300	−1.11079500	0.82070600
	B	−0.82417500	−1.80548100	−0.30755400
	B	−1.79159100	−0.48118100	−0.74073200
	La	0.75368900	0.00002500	−0.00001900
LaB_6^--Ⅱ	B	0.75876600	1.61491200	0.59962500
	B	2.07612700	1.39743800	−0.19616000
	B	2.07480900	−1.39785400	−0.19663700
	B	2.69236200	−0.00041300	−0.61748300
	B	0.75803600	−1.61500500	0.60014200
	B	1.51396400	−0.00007400	0.58976100
	La	−0.86614600	0.00008700	−0.06835500
LaB_6^--Ⅲ	B	−3.16743800	−0.00000400	−0.00042100
	B	−0.86809400	−1.61523400	0.00033200
	B	−2.41615400	−1.41485000	0.00023600
	B	−1.49439100	−0.00000200	0.00104100
	B	−0.86810400	1.61523300	0.00015600
	B	−2.41616500	1.41484600	0.00044100
	La	0.98511800	0.00000100	−0.00015700
LaB_6^--Ⅳ	B	1.48923500	0.80265400	−1.00699900
	B	1.48923300	0.80281400	1.00682600
	B	1.17566100	1.94387600	−0.00018600
	B	1.48924200	−0.80295600	1.00696400
	B	1.17493000	−1.94396500	0.00012000
	B	1.48910800	−0.80312100	−1.00696400
	La	−0.72872000	0.00006100	0.00002100

表 S2 PBE1PBE/Sc/SDD/B/6−311+G*计算水平下，ScB_6^-低能异构体的笛卡尔坐标

Table S2. Cartesian coordinates of the low−lying isomers of the ScB_6^- clusters at the PBE1PBE/Sc/SDD/B/6−311+G* level.

Cluster	Atoms	X	Y	Z
ScB_6^- − I	B	−1.02779800	1.11481300	0.81541100
	B	−0.14281100	1.75174700	−0.31553900
	B	−0.14103400	−1.75185200	0.31527200
	B	−1.15598600	0.47335000	−0.75272600
	B	−1.02699400	−1.11561900	−0.81534200
	B	−1.15520800	−0.47446600	0.75302500
	Sc	1.10710200	0.00048300	−0.00002400
ScB_6^- − II	B	−0.03208500	1.57760300	0.24921900
	B	−2.25721600	0.00004200	−0.29542600
	B	−1.53907900	1.41004400	−0.08333200
	B	−1.53912300	−1.41015900	−0.08313200
	B	−0.72342900	−0.00007100	0.39151400
	B	−0.03206500	−1.57735400	0.24906700
	Sc	1.45785700	−0.00002500	−0.10188300
ScB_6^- −III	B	0.00000000	0.69908500	0.00000000
	B	0.00232000	2.36646400	0.00000000
	B	1.57669300	0.05427000	0.00000000
	B	−1.41396400	1.60737700	0.00000000
	B	1.41681800	1.60400800	0.00000000
	B	−1.57724600	0.05787700	0.00000000
	Sc	−0.00110000	−1.52121000	0.00000000
ScB_6^- −IV	B	−1.90177500	−0.46205000	0.00000700
	B	1.90186100	−0.46193600	−0.00000400
	B	0.80411200	−0.84817200	1.02925600
	B	−0.80405500	−0.84823600	−1.02930900
	B	−0.80403600	−0.84823600	1.02930500
	B	0.80409800	−0.84812300	−1.02927600
	Sc	−0.00004900	1.02779600	0.00000500

表 S3 PBE1PBE/La/SDD/B/6−311+G*计算水平下，LaB_8^-低能异构体的笛卡尔坐标

Table S3. Cartesian coordinates of the low−lying isomers of the LaB_8^- clusters at the PBE1PBE/La/SDD/B/6−311+G* level.

Cluster	Atoms	*X*	*Y*	*Z*
LaB_8^- − I	B	1.41808900	−0.08250400	−1.62638400
	B	1.41974700	−0.08228300	1.62617500
	B	1.06905700	1.33224500	−0.98082000
	B	1.51596600	−1.40474400	−0.79501400
	B	0.02362900	2.06774300	0.00005600
	B	1.51694900	−1.40437600	0.79453300
	B	1.86844000	0.02498100	−0.00034000
	B	1.06972400	1.33219300	0.97998200
	La	−0.86856200	−0.15642600	0.00015900
	B	0.00000000	0.00000000	−1.70483500

LaB_8^--II	B	0.00000000	1.77532500	−1.39330500
	B	1.38800500	1.10689700	−1.39330500
	B	0.77028500	−1.59951300	−1.39330500
	B	−0.77028500	1.59951300	−1.39330500
	B	−1.38800500	1.10689700	−1.39330500
	B	−1.73081400	−0.39504700	−1.39330500
	B	1.73081400	−0.39504700	−1.39330500
	La	0.00000000	0.00000000	1.00508500
LaB_8^--III	B	−1.21551000	−0.00004000	−0.63044800
	B	−0.72551800	1.77502100	−0.25846100
	B	−1.23187500	0.77340000	0.99631000
	B	−2.28005100	1.46148900	−0.31053700
	B	−2.28009300	−1.46149400	−0.31044600
	B	−0.72544600	−1.77491800	−0.25862900
	B	−2.86301300	−0.00000900	−0.03637300
	B	−1.23174800	−0.77348900	0.99640900
	La	1.10116300	0.00000300	−0.01647600
LaB_8^--IV	B	0.71300000	−0.02715800	1.29738700
	B	2.23870100	−0.22371700	0.89627600
	B	2.43475000	−1.29829500	−0.47981600
	B	3.13040400	0.12116200	−0.53360200
	B	2.30776000	1.42025700	−0.14849700
	B	1.27051500	0.08404500	−0.63441400
	B	0.97013200	−1.43913300	0.16651700
	B	0.71240300	1.54129300	0.11079000
	La	−1.20856700	−0.01565400	−0.05917900

表 S4 PBE1PBE/Sc/SDD/B/6−311+G*计算水平下，ScB_8^-低能异构体的笛卡尔坐标

Table S4. Cartesian coordinates of the low−lying isomers of the ScB_8^- clusters at the PBE1PBE/Sc/SDD/B/6−311+G* level.

Cluster	Atoms	*X*	*Y*	*Z*
ScB_8^--I	B	−0.63675500	−1.77085200	−0.12114200
	B	−0.65938400	−1.00452800	−1.46461800
	B	−0.64339900	1.64588800	−0.65089800
	B	−0.68514200	−1.20691800	1.30537400
	B	−1.04527800	−0.00438000	−0.00114900
	B	−0.67488600	0.50990800	−1.69911800
	B	−0.70046800	1.53974400	0.88078600
	B	−0.62860300	0.26932100	1.74961300
	Sc	1.35093200	0.00519400	0.00027400
ScB_8^--II	B	−1.68054500	0.33763600	−0.78894900
	B	−0.66754600	−0.50324200	1.62649200
	B	1.81259000	−0.79322400	−0.00009600
	B	−0.89408500	−0.93610900	−0.00014300
	B	−0.66752500	−0.50277200	−1.62665000
	B	−1.68057000	0.33740900	0.78904500
	B	0.65372600	−1.12859100	−1.04129800

	B	0.65372500	−1.12888700	1.04101000
	Sc	0.58815000	1.02804300	0.00014000
ScB_8^--III	B	0.00000000	2.02629800	−0.44509600
	B	2.02629800	0.00000000	−0.44509600
	B	−1.43280900	−1.43280900	−0.44509600
	B	0.00000000	−2.02629800	−0.44509600
	B	1.43280900	1.43280900	−0.44509600
	B	−2.02629800	0.00000000	−0.44509600
	B	1.43280900	−1.43280900	−0.44509600
	B	−1.43280900	1.43280900	−0.44509600
	Sc	0.00000000	0.00000000	0.84780100
ScB_8^--IV	B	0.47014200	−0.77097200	0.98835100
	B	0.51052700	−0.00003200	−0.64452300
	B	−0.04200900	−1.70612600	−0.34097300
	B	1.52622600	1.46078100	−0.29652000
	B	0.47018700	0.77093200	0.98833100
	B	−0.04200800	1.70609000	−0.34096100
	B	2.09765400	0.00001500	0.05136400
	B	1.52622500	−1.46074400	−0.29652900
	Sc	−1.55165300	0.00001400	−0.02584300

补充材料 B: REB_n^- (RE = La, Sc; *n* = 6, 8) 团簇低能异构体的对称性, 相对能和第一垂直拆分能

Suppl. B: Symmetry, relative energies, and first VDE of low-lying isomers of REB_n^- (RE = La, Sc; *n* = 6, 8)

表 S5 REB_n^- (RE = La, Sc; *n* = 6, 8) 团簇低能异构体的对称性, 相对能和第一垂直拆分能 (VDE)

Table S5. Symmetry, relative energies, and first VDE of low-lying isomers of REB_n^- (RE = La, Sc; *n* = 6, 8).

Cluster	lsomers	Sym.	Δ*E* /eV	VDE/eV
LaB_6^-	I	C_2	0.00	1.74
	II	C_s	0.06	1.89
	III	C_{2v}	0.19	2.36
	IV	C_{2v}	0.86	1.66
ScB_6^-	I	C_2	0.00	2.08
	II	C_2	0.03	1.92
	III	C_{2v}	0.05	1.91
	IV	C_{2v}	0.57	1.93
LaB_8^-	I	C_s	0.00	2.29
	II	C_{7v}	0.43	1.24
	III	C_s	1.40	2.04
	IV	C_1	1.52	2.02
ScB_8^-	I	C_{7v}	0.00	1.91
	II	C_s	0.30	2.45
	III	C_{8v}	1.22	1.71
	IV	C_s	1.54	3.22

