Electronic supplementary material

Comparison of DAFH and FALDI-like approaches

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Section S1.   Geometry for B_2H_6

Table S1   Cartesian coordinates (in Å) used for symmetry-unique atoms in B_2H_6 (D_{2h}), with the inversion center taken as the origin. H_b is a bridging H atom and H_t is a terminal one.

Atom	x	y	z
B	0.888375	0	0
H_b	0	0	0.973751
H_t	1.463157	1.035737	0

Section S2.   Additional results for H_2

Figure S1.   Dominant DAFH functions associated with the domain of one of the H atoms in H_2 at three representative nuclear separations, generated using the one-electron approximation. Also shown for each function is the corresponding occupation number as well as the proportion of $k_{HH'} = \frac{1}{2}\,\text{SEDI}(H, H')$ which can be assigned to a term P_i (see equation 6) that involves this function.
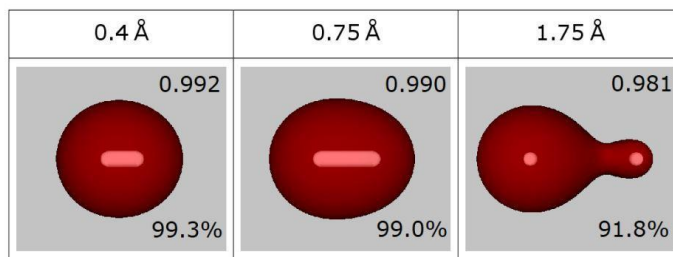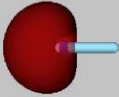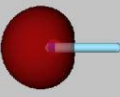
Figure S2.   Dominant FALDI-like functions associated with the domain of one of the H atoms in H_2 at three representative nuclear separations, together with their eigenvalues and relative contributions to the relevant k values, calculated using the one-electron approximation. For each of these values of R, the first row corresponds to partitioning of k_{HH} and the second one to partitioning of $k_{HH'}$. Columns are labelled A-D according to the variant of the approach, as described in the text.
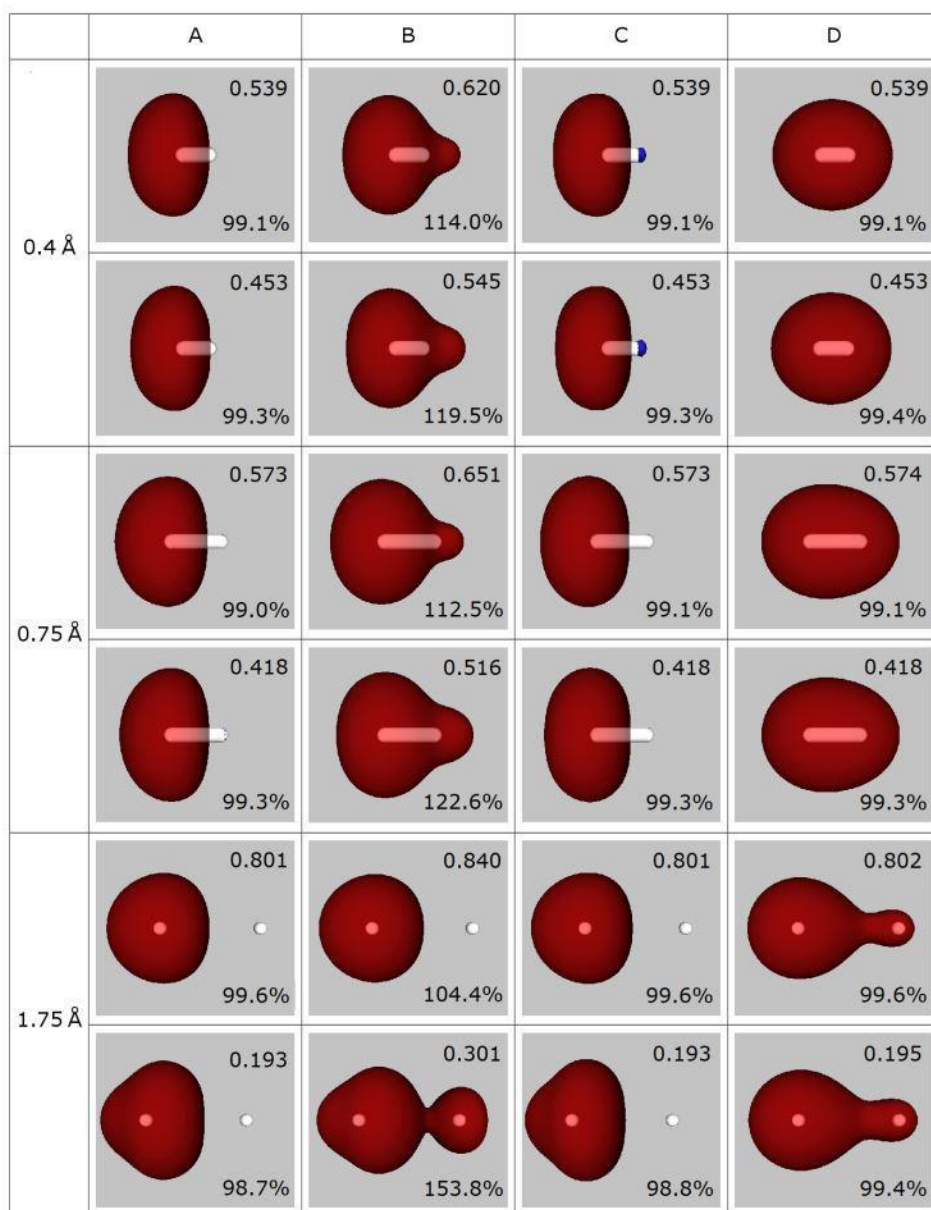
Section S3.   Additional results for N₂

Figure S3.   Dominant DAFH functions associated with the domain of one of the N atoms in N_2 at three representative nuclear separations, generated using the one-electron approximation. Also shown for each function is the corresponding occupation number as well as the proportion of $k_{NN'} = \frac{1}{2} \, SEDI(N, N')$ which can be assigned to a term P_i (see equation 6) that involves this function.
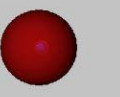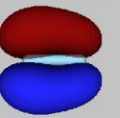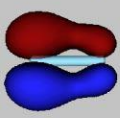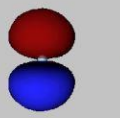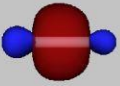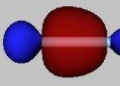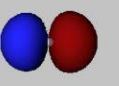
Figure S4.   Dominant Scheme B FALDI-like functions that can be associated (by visual inspection) with the domain of one of the N atoms in N_2 at three representative nuclear separations, together with their eigenvalues and relative contributions to the relevant k values, generated using the full calculation.
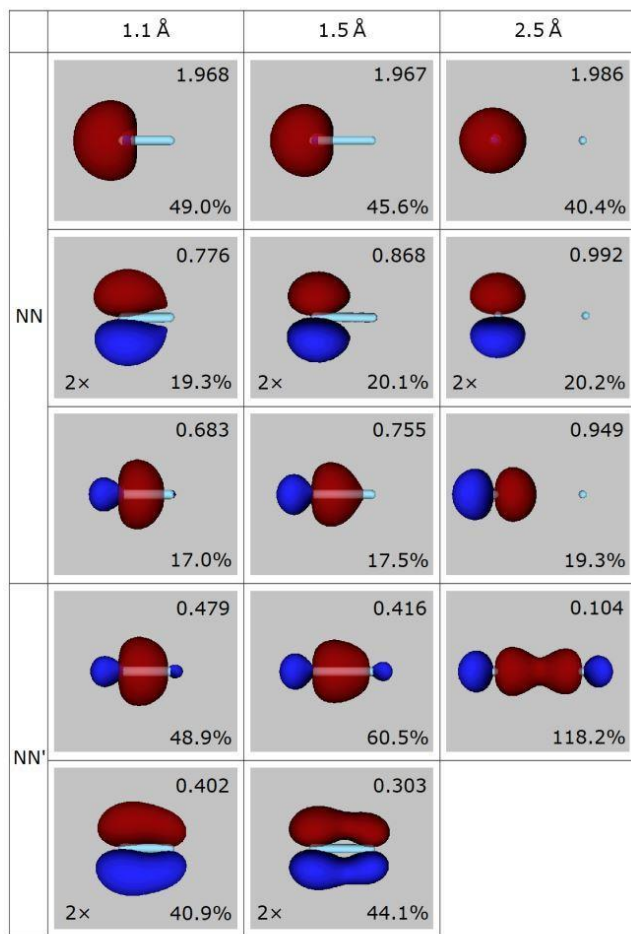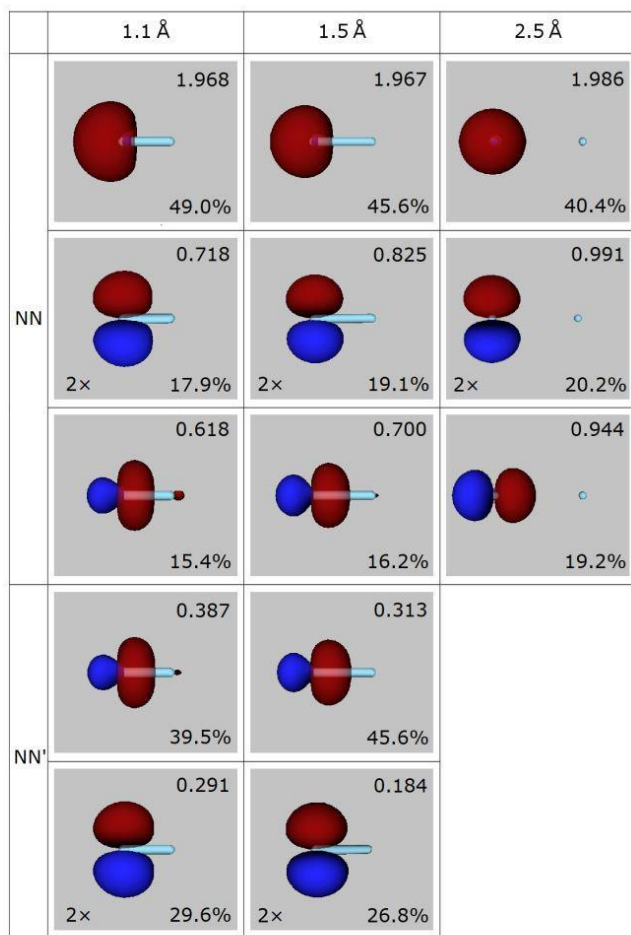
Figure S5. Dominant Scheme C FALDI-like functions that can be associated (by visual inspection) with the domain of one of the N atoms in N_2 at three representative nuclear separations, together with their eigenvalues and relative contributions to the relevant k values, generated using the full calculation.
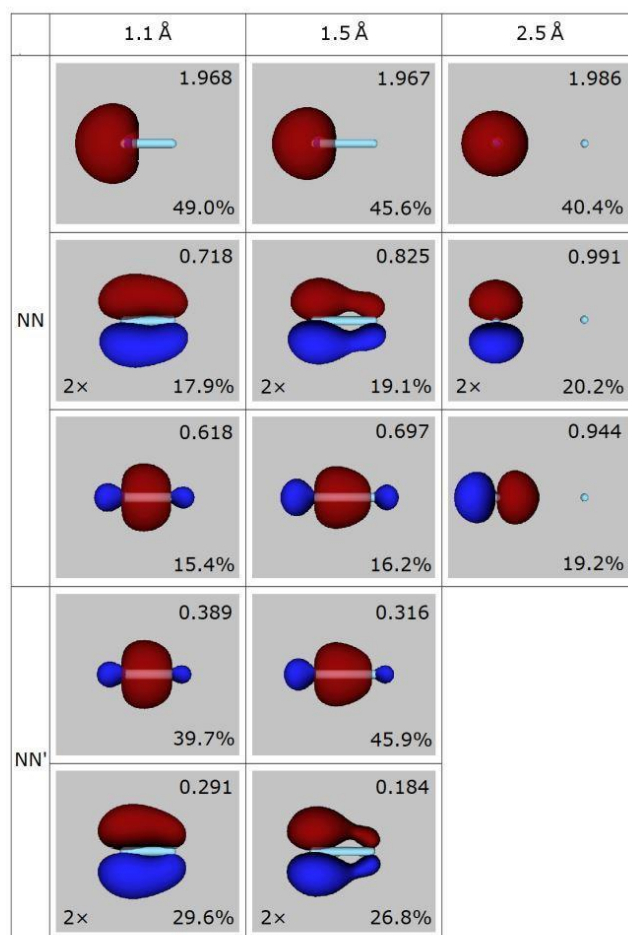
Figure S6. Dominant Scheme D FALDI-like functions that can be associated (by visual inspection) with the domain of one of the N atoms in N_2 at three representative nuclear separations, together with their eigenvalues and relative contributions to the relevant k values, generated using the full calculation.

Figure S7.   Dominant Scheme A FALDI-like functions that can be associated (by visual inspection) with the domain of one of the N atoms in N_2 at three representative nuclear separations, together with their eigenvalues and relative contributions to the relevant k values, calculated using the one-electron approximation.
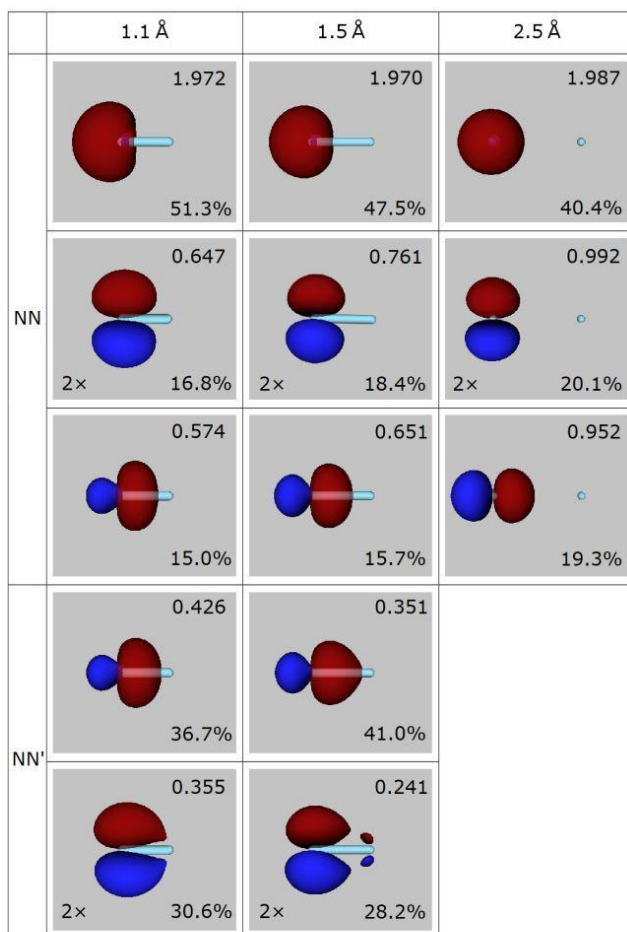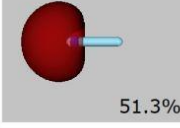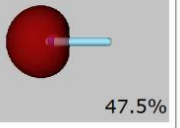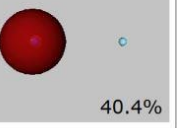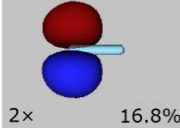
	1.1 Å	1.5 Å	2.5 Å
NN	1.972 ... 51.3%	1.970 ... 47.5%	1.987 ... 40.4%
	2× 0.647 ... 16.8%	2× 0.761 ... 18.4%	2× 0.992 ... 20.1%
	0.574 ... 15.0%	0.651 ... 15.7%	0.952 ... 19.3%
NN'	0.426 ... 36.7%	0.351 ... 41.0%	
	2× 0.355 ... 30.6%	2× 0.241 ... 28.2%	

Figure S8.   Dominant Scheme B FALDI-like functions that can be associated (by visual inspection) with the domain of one of the N atoms in N_2 at three representative nuclear separations, together with their eigenvalues and relative contributions to the relevant k values, calculated using the one-electron approximation.
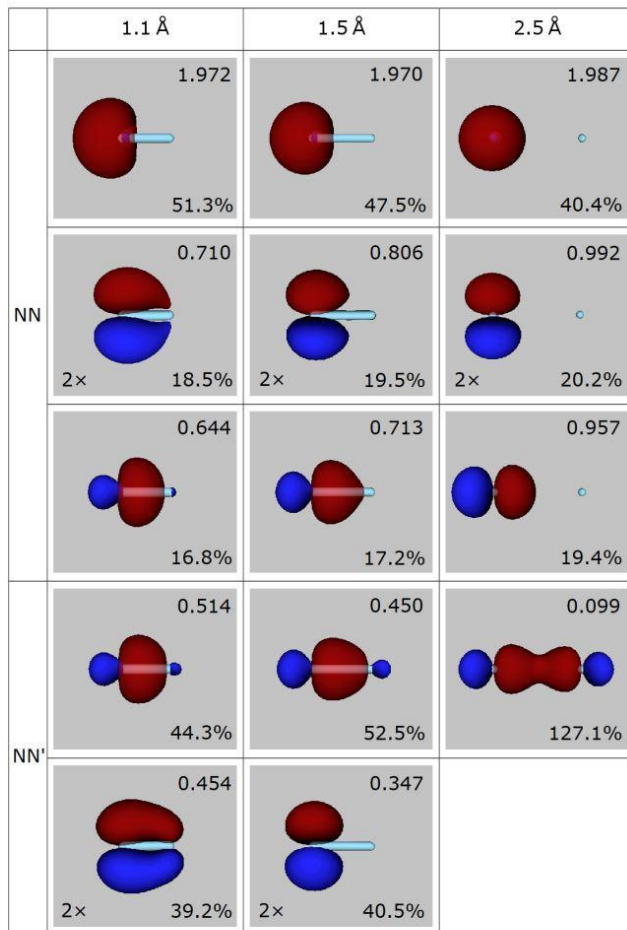
Figure S9.   Dominant Scheme C FALDI-like functions that can be associated (by visual inspection) with the domain of one of the N atoms in N_2 at three representative nuclear separations, together with their eigenvalues and relative contributions to the relevant k values, calculated using the one-electron approximation.

Figure S10. Dominant Scheme D FALDI-like functions that can be associated (by visual inspection) with the domain of one of the N atoms in N_2 at three representative nuclear separations, together with their eigenvalues and relative contributions to the relevant k values, calculated using the one-electron approximation.
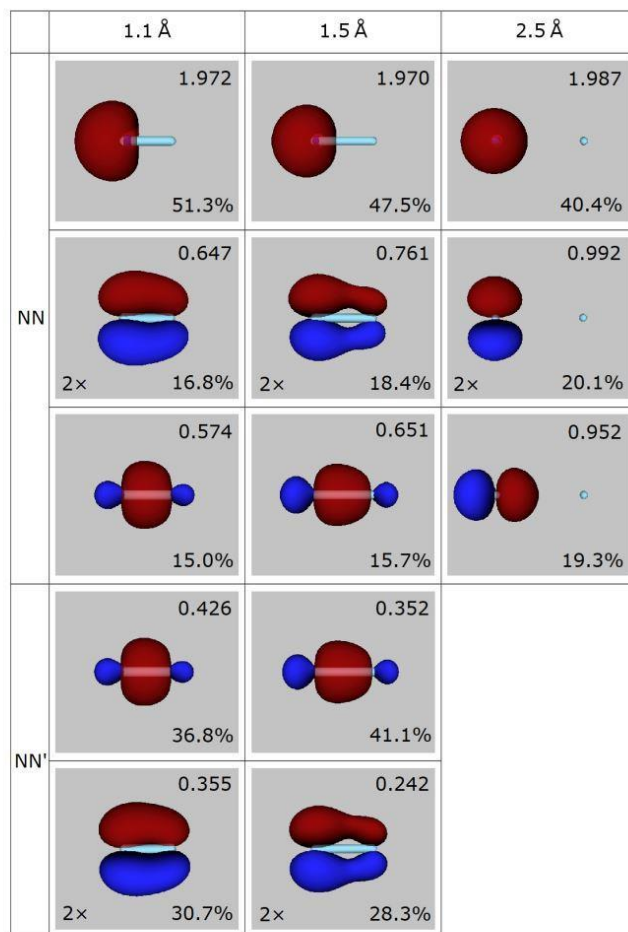
Section S4. Additional results for B_2H_6

Figure S11. Dominant DAFH functions (first column) and Scheme B FALDI-like functions (second and third columns) for B_2H_6, together with their eigenvalues and relative contributions to relevant k values, generated using the full calculation. The specific domains used for each of these functions are the same as those in Figure 5 and are identified in the main text, expect that the additional function depicted in the third column is associated with one of the B domains.
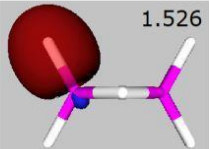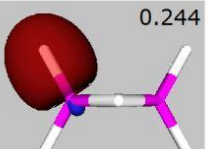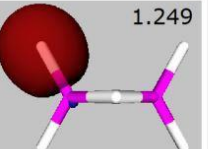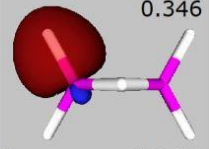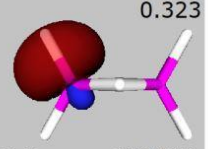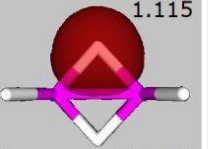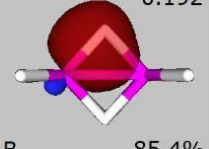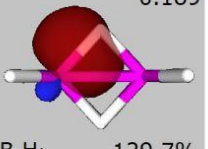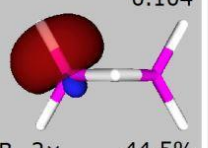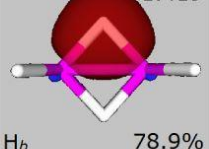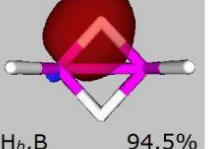
Figure S12. Dominant DAFH functions (first column) and Scheme C FALDI-like functions (second and third columns) for B_2H_6, together with their eigenvalues and relative contributions to relevant k values, generated using the full calculation. The specific domains used for each of these functions are the same as those in Figure 5 and are identified in the main text.

Figure S13. Dominant DAFH functions (first column) and Scheme D FALDI-like functions (second and third columns) for B_2H_6, together with their eigenvalues and relative contributions to relevant k values, generated using the full calculation. The specific domains used for each of these functions are the same as those in Figure 5 and are identified in the main text.
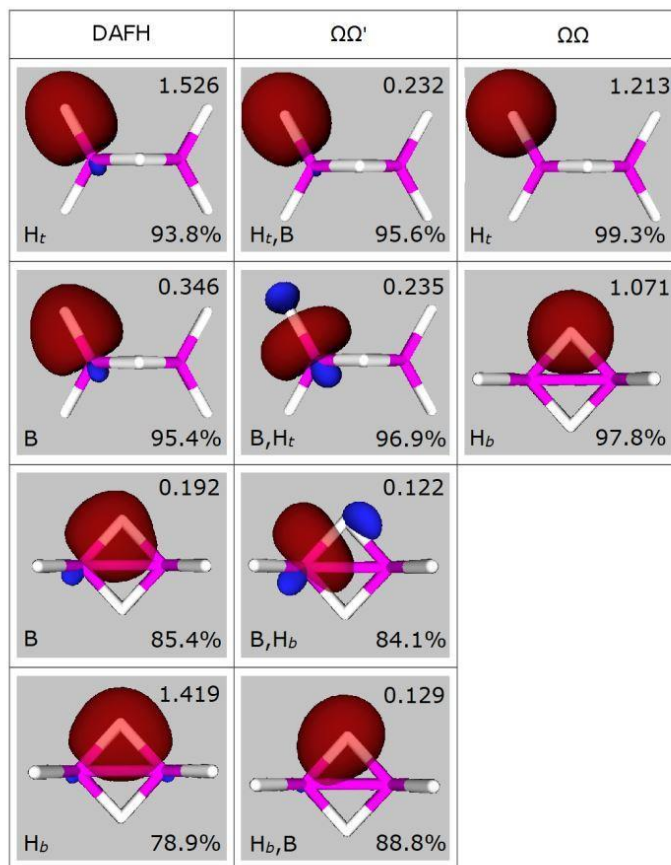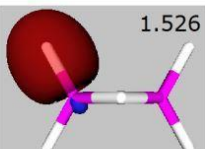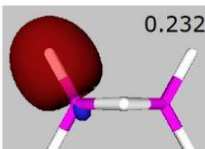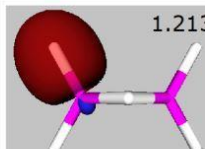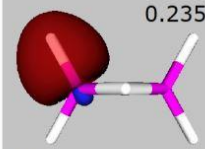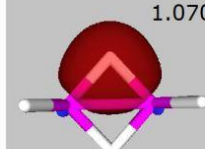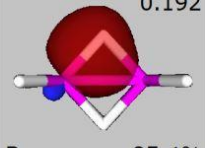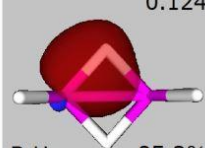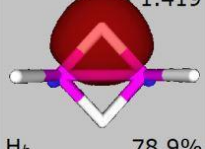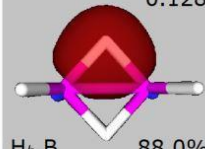
Figure S14. Dominant DAFH functions (first column) and Scheme A FALDI-like functions (second and third columns) for B_2H_6, together with their eigenvalues and relative contributions to relevant k values, calculated using the one-electron approximation. The specific domains used for each of these functions are the same as those in Figure 5 and are identified in the main text.
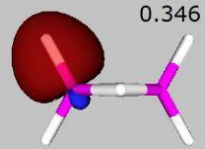
Figure S15. Dominant DAFH functions (first column) and Scheme B FALDI-like functions (second and third columns) for B_2H_6, together with their eigenvalues and relative contributions to relevant k values, calculated using the one-electron approximation. The specific domains used for each of these functions are the same as those in Figure 5 and are identified in the main text.

Figure S16. Dominant DAFH functions (first column) and Scheme C FALDI-like functions (second and third columns) for B_2H_6, together with their eigenvalues and relative contributions to relevant k values, calculated using the one-electron approximation. The specific domains used for each of these functions are the same as those in Figure 5 and are identified in the main text.
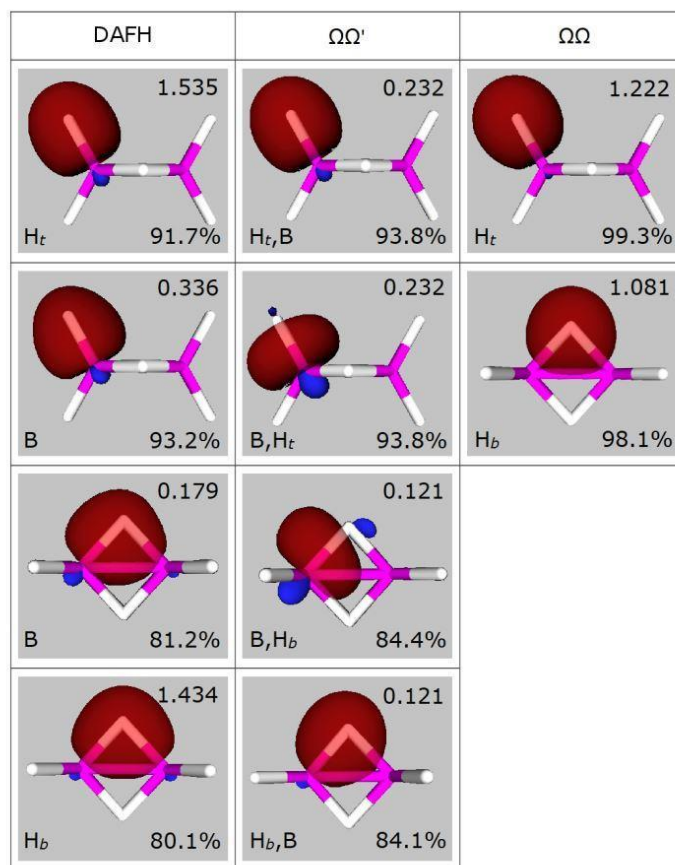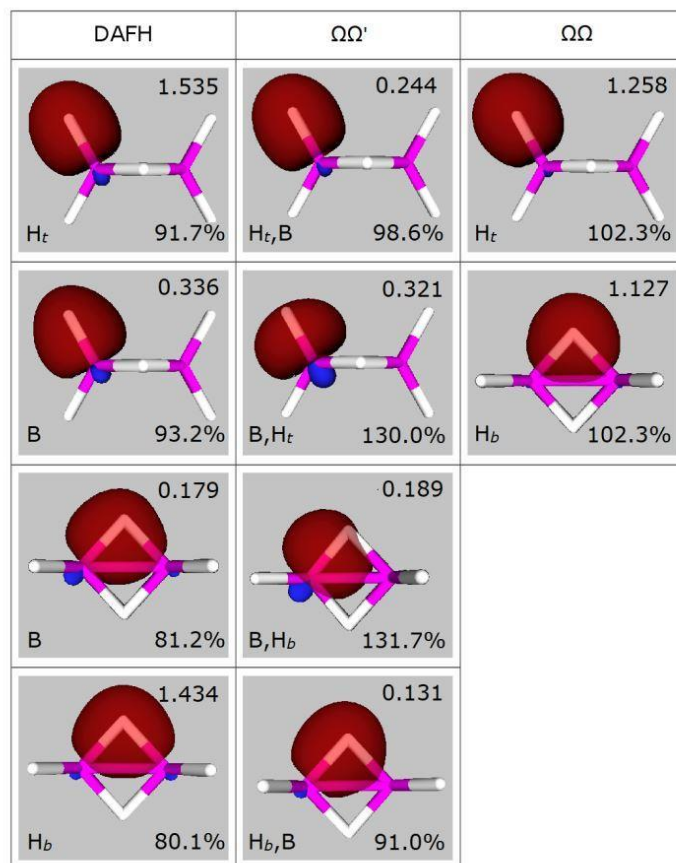
Figure S17. Dominant DAFH functions (first column) and Scheme D FALDI-like functions (second and third columns) for B_2H_6, together with their eigenvalues and relative contributions to relevant k values, calculated using the one-electron approximation. The specific domains used for each of these functions are the same as those in Figure 5 and 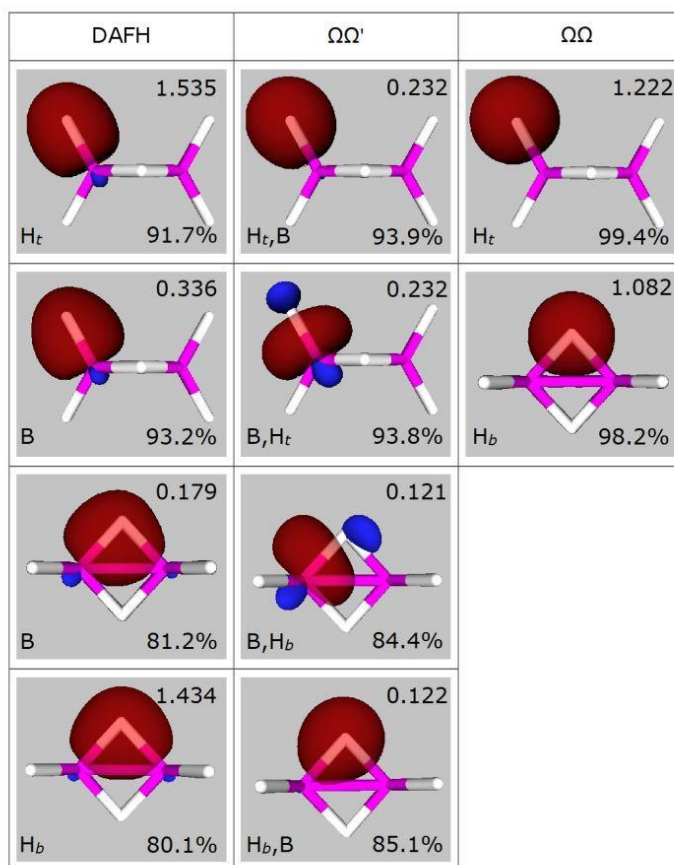are identified in the main text.