Supplementary Materials: Computational Modelling of Pyrrolic MN_4 Motifs Embedded in Graphene for Catalyst Design

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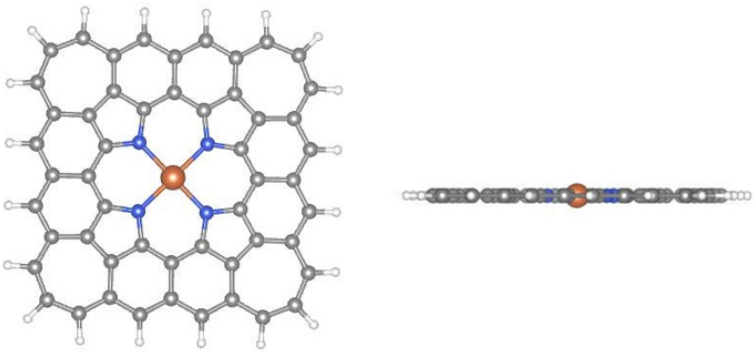
Contents

1. Structural Data

The structural data for FeN_4 clusters and unit cells. For each cluster, the top and side views are shown. Cluster geometries are given in xyz format and unit cell geometries are given in VASP POSCAR format.

1.1. FeN_4, Pyrrolic-1



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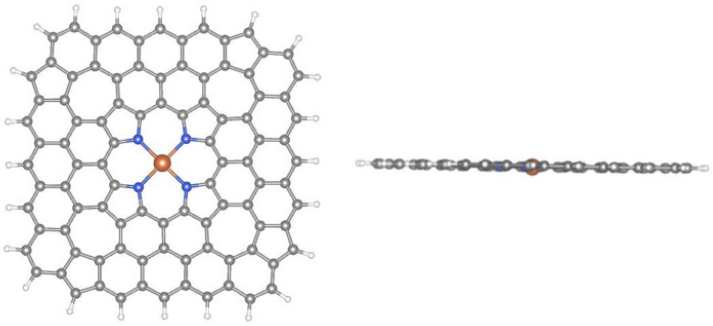

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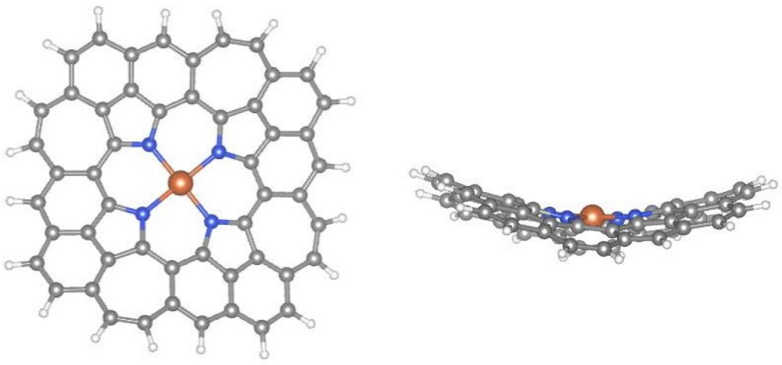

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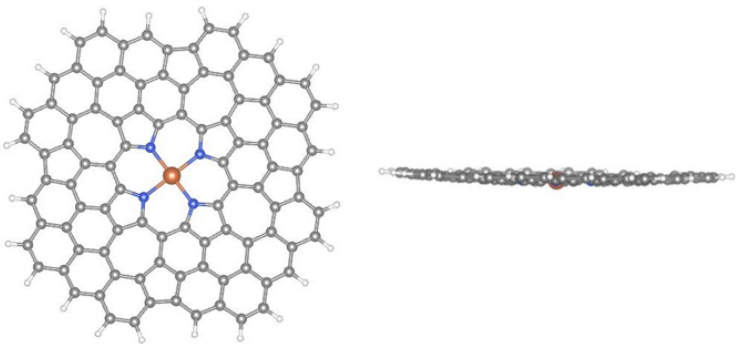
1.4. FeN_4, Pyrrolic-2L



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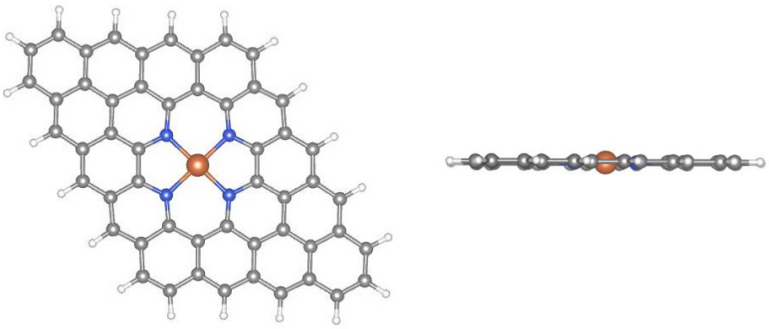

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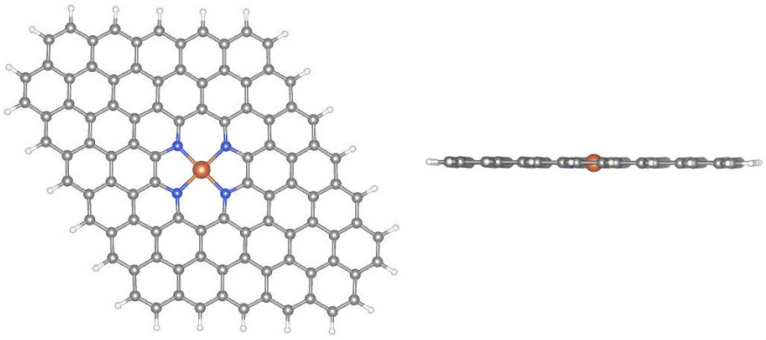

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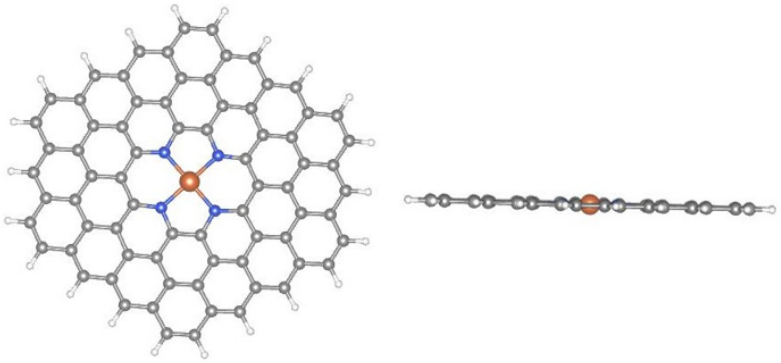

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C	2.4213514	7.7257998	-0.0019254
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H	9.4106938	-2.3207857	1.4955186
H	7.8356457	-4.3005297	1.2749233
H	6.2497107	-6.2254237	1.0501055
H	4.7220935	-8.1063158	0.8339938
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H	0.0597765	-8.6287144	0.0362869
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H	-2.3167360	-8.3074946	-0.3855239
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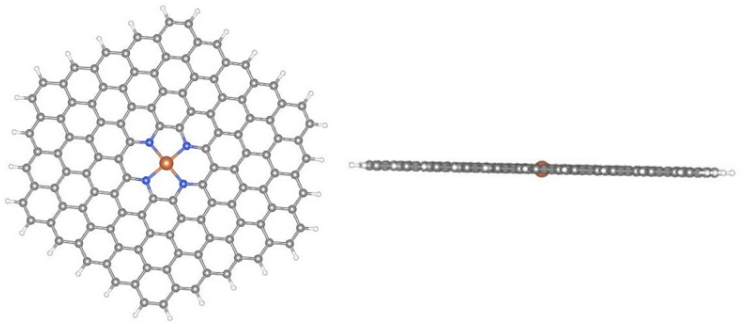
1.8. FeN_4, Pyridinic-2L



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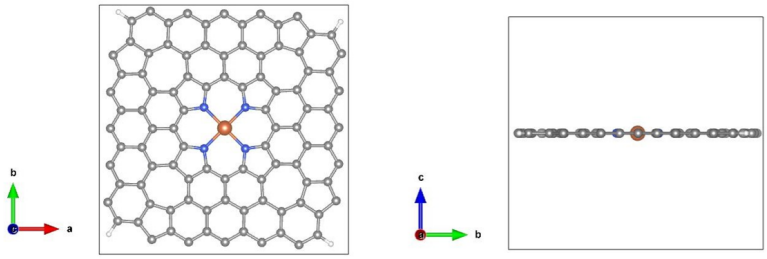
1.9. FeN_4, Pyrrolic-UC1

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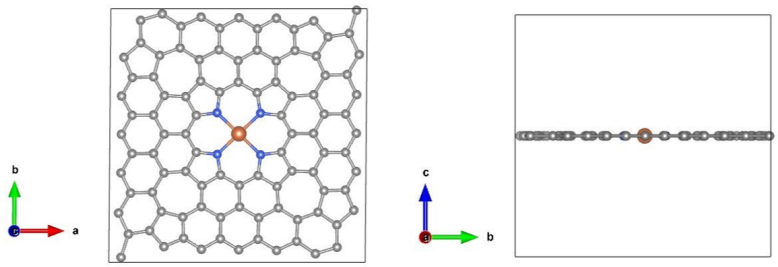
1.10. FeN_4, Pyrrolic-UC1b

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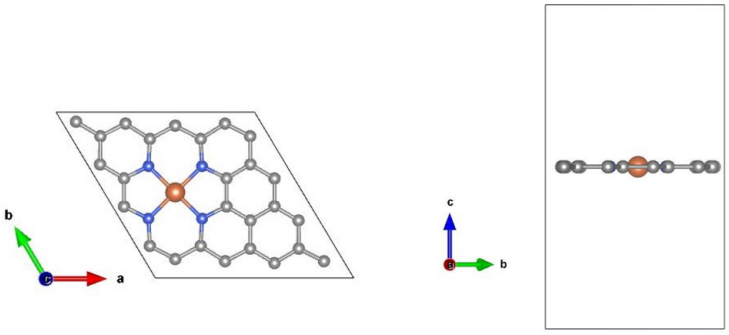
1.11. FeN_4, Pyridinic-UC

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2. Non-planar MN_4 binding

In this section, the top view and side view of non-planar binding motifs discussed in Table 2 are shown. Planar pyrrolic TiN_4 and VN_4 are additionally included for comparison with pyridinic motifs.

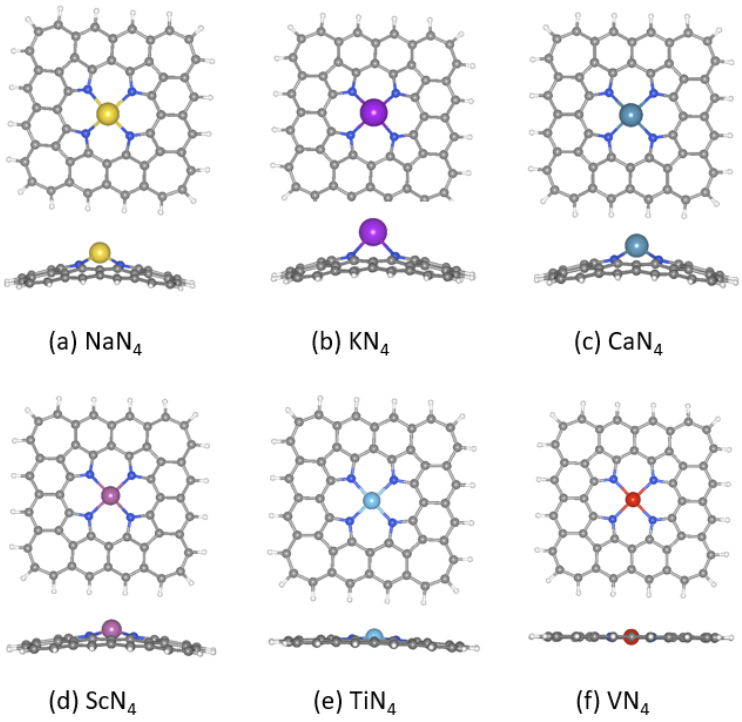

Figure S1. (a-d) Top and side views of pyrrolic-1 MN_4 clusters with non-planar binding geometries. (e,f) Ti and V are included for comparison with pyridinic structures.

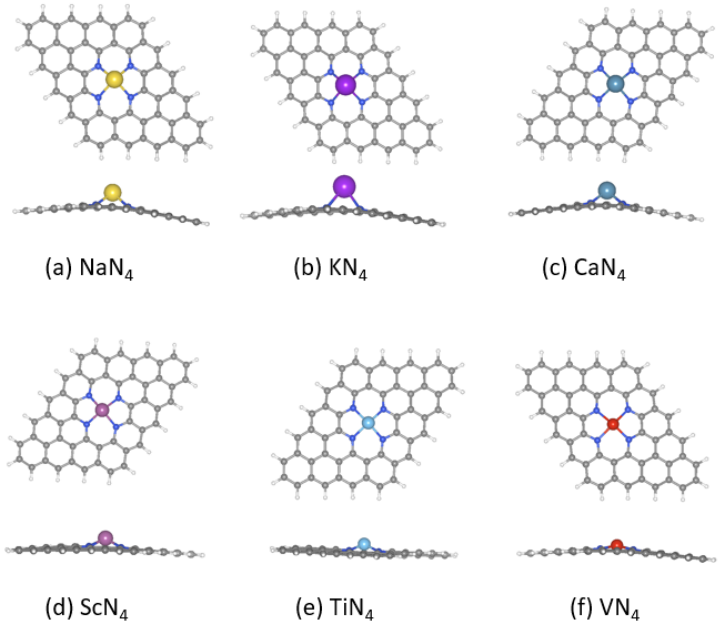

Figure S2. Top and side views of pyridinic-1 MN_4 clusters with non-planar binding geometries.

3. Frontier Molecular Orbitals of Fe and Zn

In this section, the frontier molecular orbitals are plotted to illustrate the differences in binding character between a highly ionic binding character (Zn) and a binding situation involving π-d interaction (Fe). For the pyrrolic-1 FeN_4 cluster, π-d interactions can be observed in all the occupied orbitals shown. In pyridinic-1 FeN_4 cluster, the orbitals illustrating π-d interactions are lower in energy. No significant π-d interaction can be observed for Zn. All orbitals are plotted with Molden.

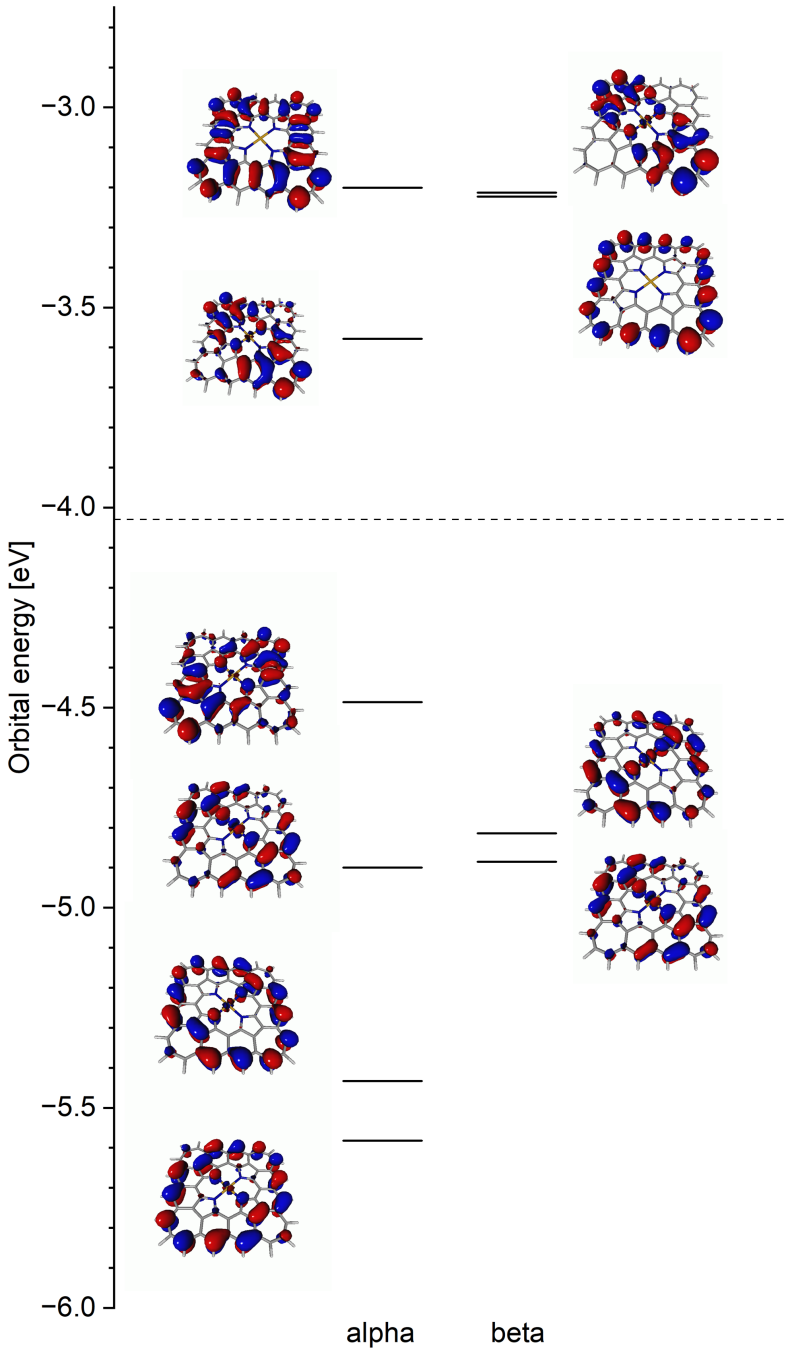

Figure S3. Frontier molecular orbitals of FeN_4 in pyrrolic-1 cluster obtained with PBE0-D3(BJ)/def2-TZVP method. Orbitals below the dashed line are occupied.

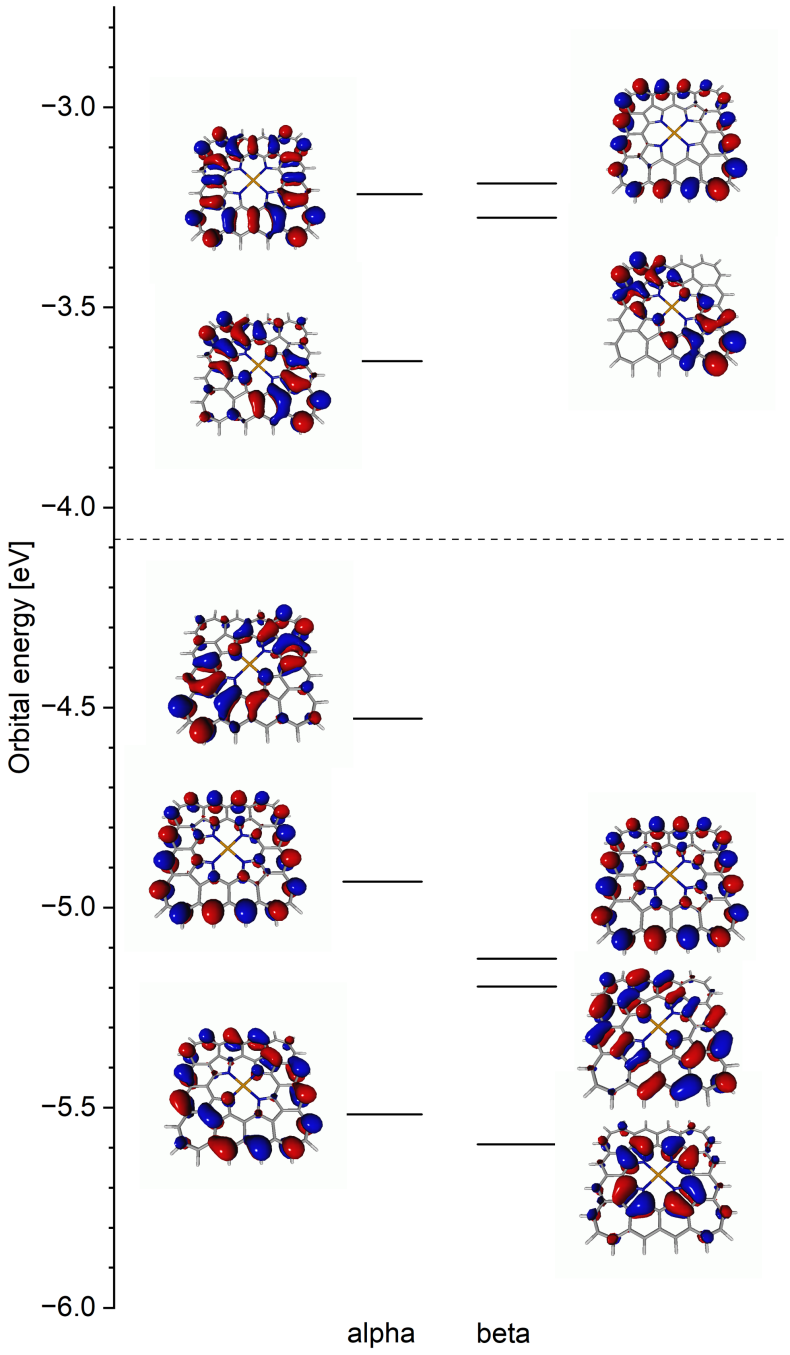

Figure S4. Frontier molecular orbitals of ZnN_4 in pyrrolic-1 cluster obtained with PBE0-D3(BJ)/def2-TZVP method. Orbitals below the dashed line are occupied.

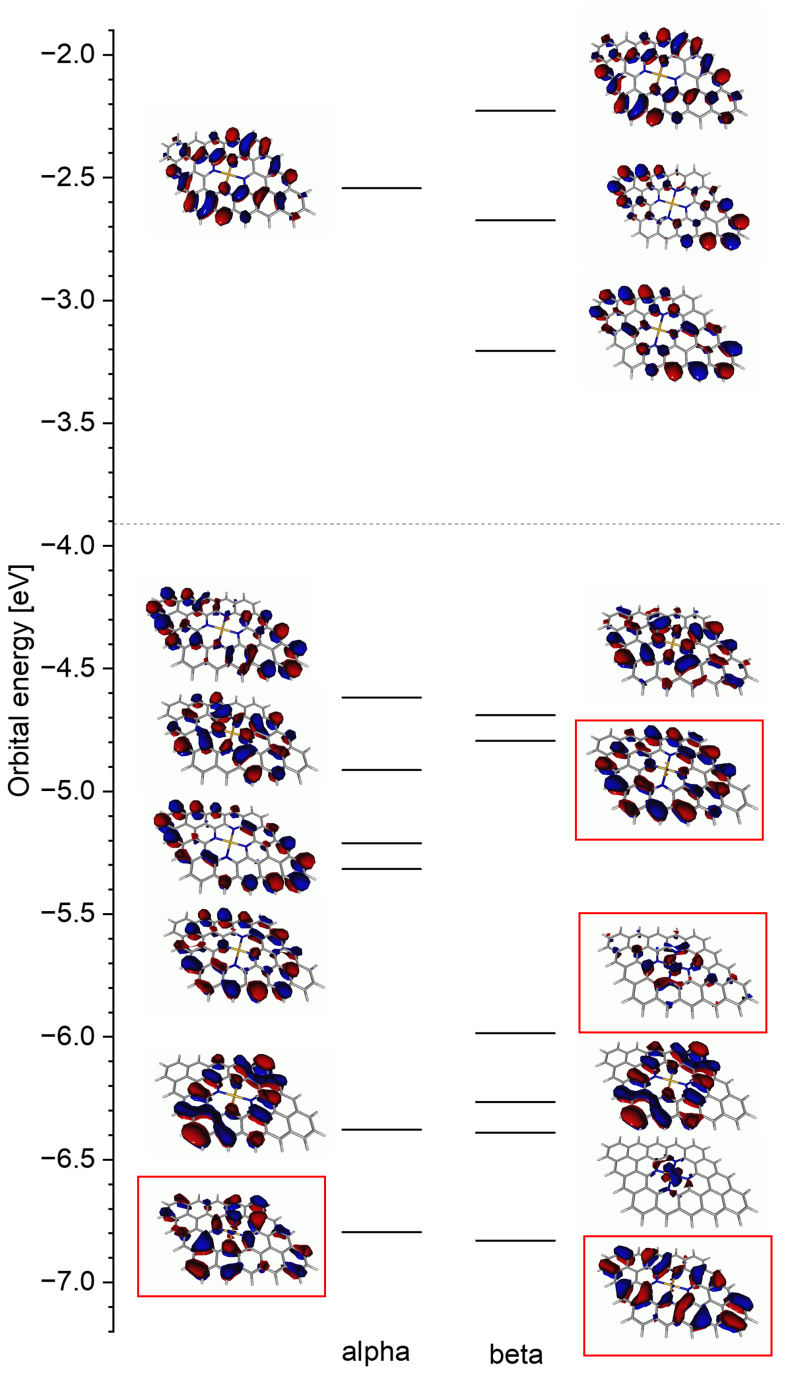

Figure S5. Frontier molecular orbitals of FeN_4 in pyridinic-1 cluster obtained with PBE0-D3(BJ)/def2-TZVP method. Orbitals which indicate π-d interactions are highlighted. Orbitals below the dashed line are occupied.

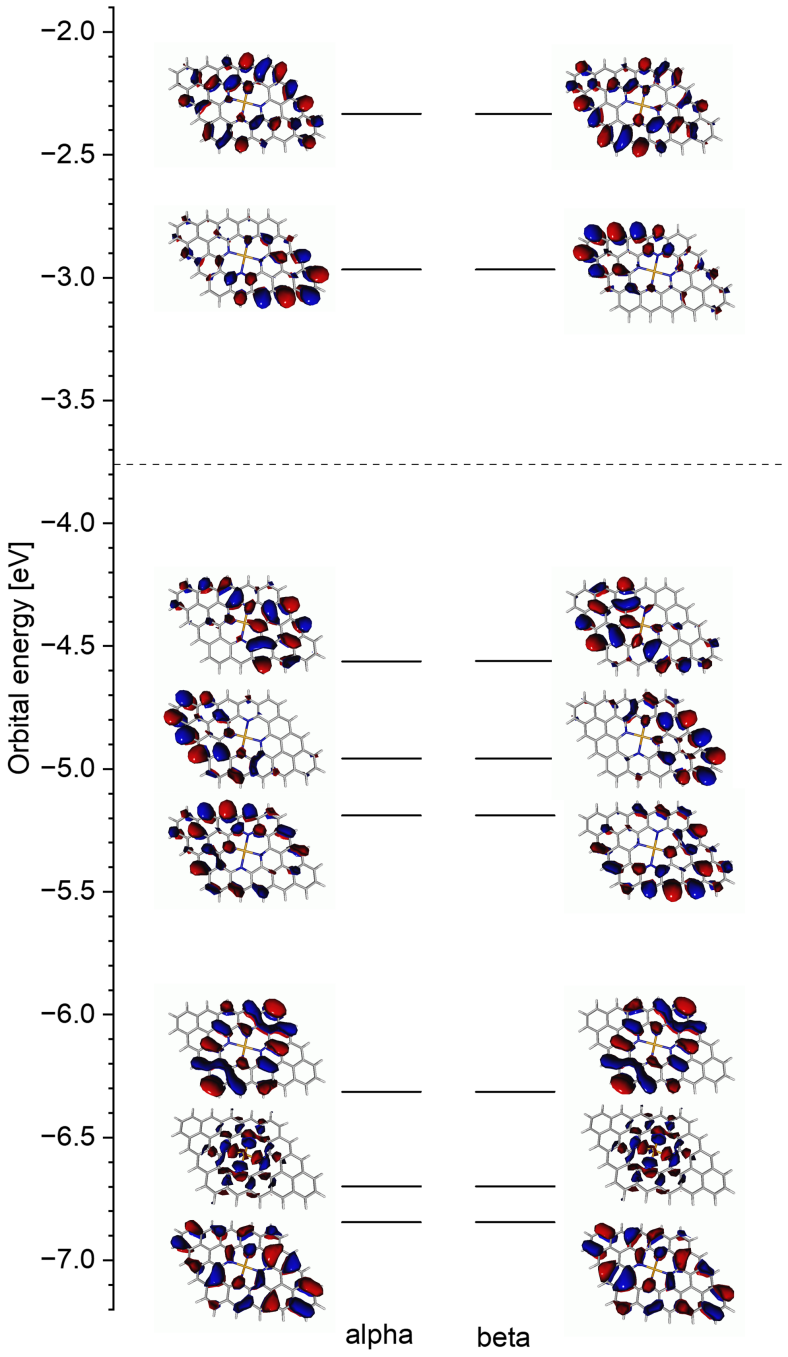

Figure S6. Frontier molecular of ZnN_4 in pyridinic-1 cluster obtained with PBE0-D3(BJ)/def2-TZVP method. Orbitals below the dashed line are occupied.