Supplemental Material: Predicted Pressure-Induced High-Energy-Density Iron Pentazolate Salts

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Table S1: The lattice parameters and atomic positions of *Fdd*2-FeN_{10}, *P*-1(No.1)-FeN_{10} and *P*-1(No.2)-FeN_{10} under ambient pressure.

Space group	Lattice parameters	Atomic coordinates (fractional)
*Fdd*2	a=10.748, b=8.910, c=8.463 α=90.0, β=90.0, γ=90.0	Fe (0.500, 0.500, 0.271) N (0.372, 0.923, 0.246) (0.257, 0.082, 0.364) (0.507, 0.346, 0.443) (0.683, 0.001, 0.769) (0.122, 0.220, 0.099)
P-1(No.1)	a=5.229, b=5.373, c=6.687 α=91.322, β=110.802, γ=119.586	Fe (0.000, 0.000, 0.000) N (0.181, 0.924, 0.294) (0.302, 0.370, 0.243) (0.598, 0.981, 0.798) (0.880, 0.859, 0.681) (0.524, 0.706, 0.829)
P-1(No.2)	a=3.959, b=3.961, c=7.201 α=96.630, β=103.731, γ=99.842	Fe (0.000, 0.500, 0.000) N (0.644, 0.775, 0.898) (0.435, 0.076, 0.681) (0.705, 0.355, 0.179) (0.284, 0.934, 0.177) (0.823, 0.183, 0.320)

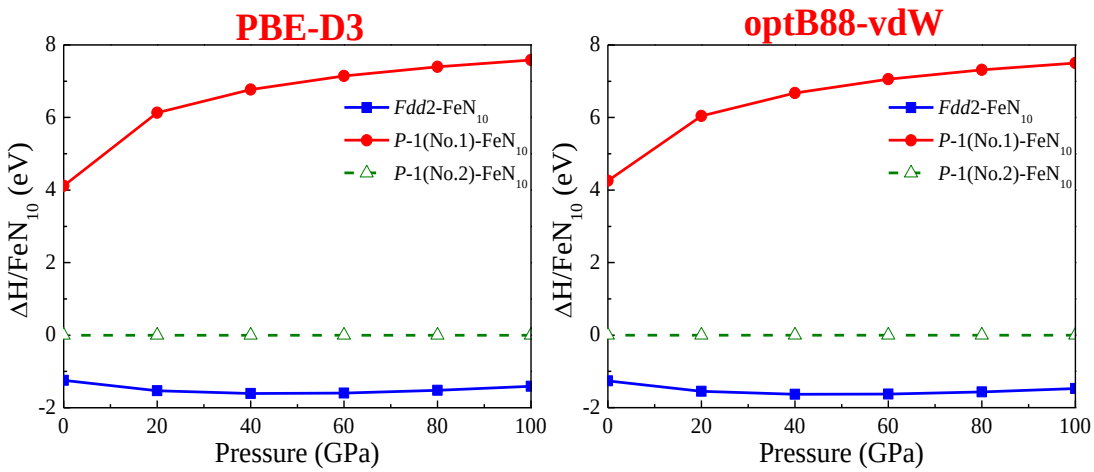

Figure S1: Relative enthalpies of *Fdd*2-FeN_{10}, *P*-1(No.1)-FeN_{10} and *P*-1(No.2)-FeN_{10} under different van der Waals correction methods (PBE-D3 and optB88-vdW). The enthalpy of *P*-1(No.2)-FeN_{10} is used as the reference state.

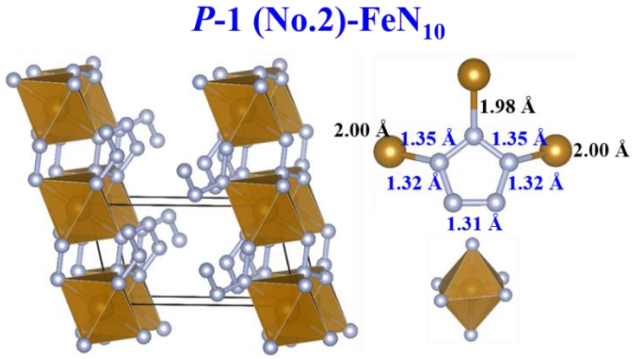

Figure S2: The crystal structure and bond lengths (Fe-N: black, N-N: blue) of *P*-1(No.2)-FeN_{10} at 0 GPa.

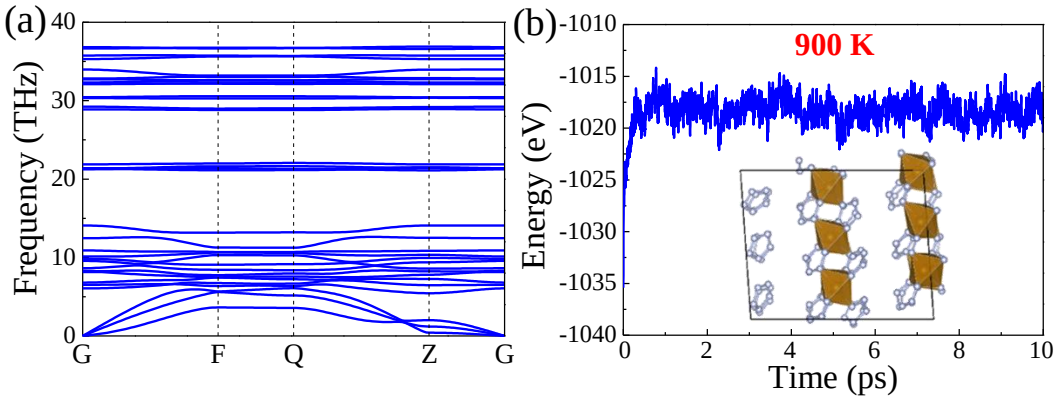

Figure S3: (a) Phonon dispersion curves *P*-1(No.2)-FeN_{10} at 0 GPa. (b) Total free energy fluctuations of *P*-1(No.2)-FeN_{10} at 900 K under ambient pressure. The illustration shows structural snapshots of *P*-1(No.2)-FeN_{10} after 10 ps in AIMD simulations.

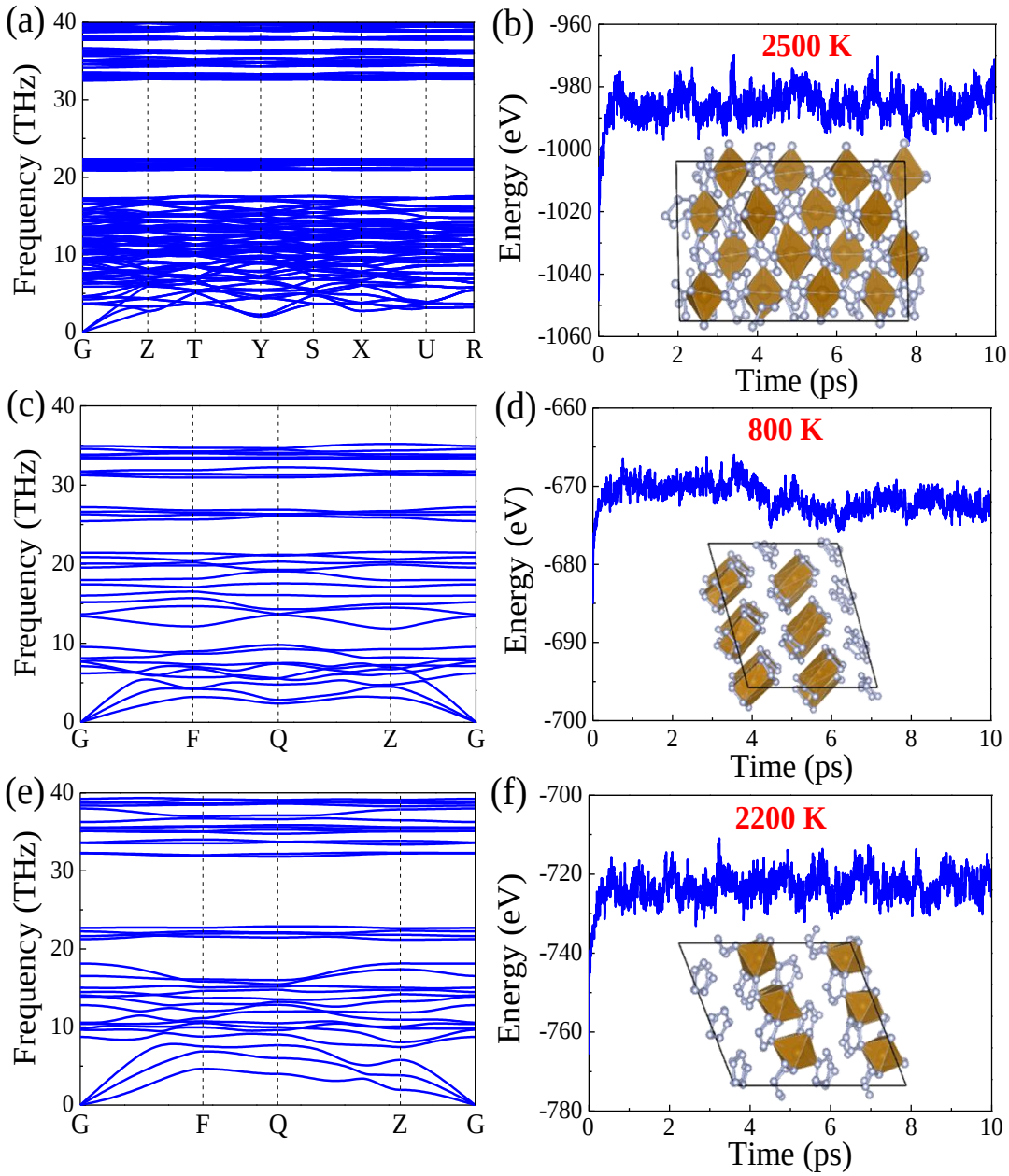

Figure S4: (a) (c) (e) Phonon dispersion curves of *Fdd*2-FeN_{10}, *P*-1(No.1)-FeN_{10} and *P*-1(No.2)-FeN_{10} at 40 GPa. (b) (d) (f) Total free energy fluctuations of *Fdd*2-FeN_{10}, *P*-1(No.1)-FeN_{10} and *P*-1(No.2)-FeN_{10} in AIMD simulations. 2500 K, 800 K and 2200 K are the highest temperature at which *Fdd*2-FeN_{10}, *P*-1(No.1)-FeN_{10} and *P*-1(No.2)-FeN_{10} can remain stable at 40 GPa respectively, and the illustrations show their structural snapshots after 10 ps.

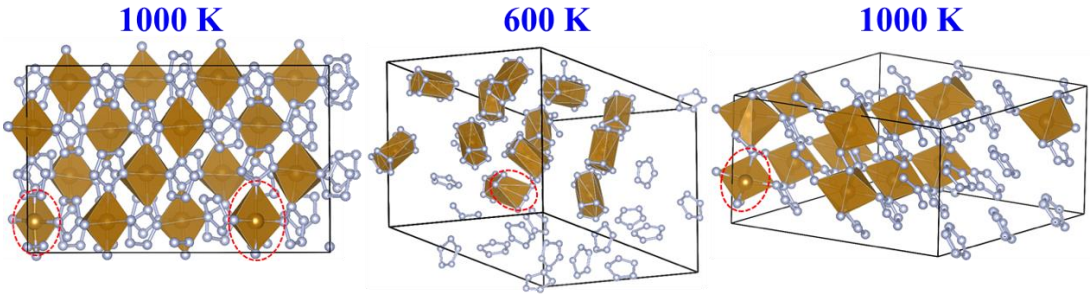

Figure S5: Temperatures and snapshots of *Fdd*2-FeN_{10}, *P*-1(No.1)-FeN_{10} and *P*-1(No.2)-FeN_{10} losing stability in AIMD simulations under ambient pressure.

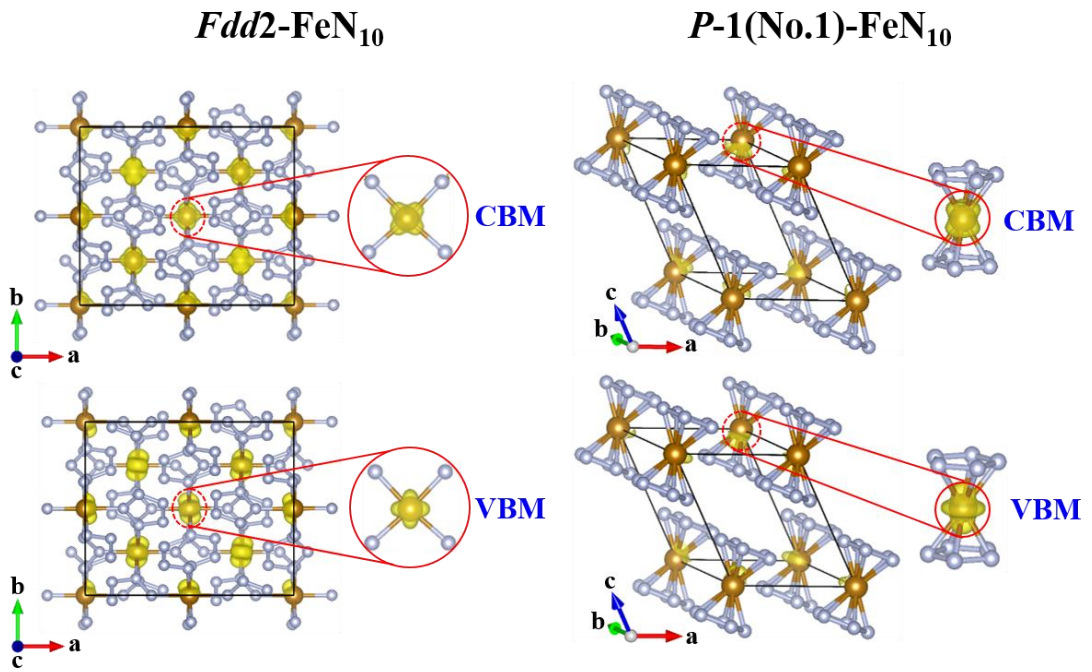

Figure S6: The partial charges of *Fdd*2-FeN_{10} and *P*-1(No.1)-FeN_{10} at ambient pressure.

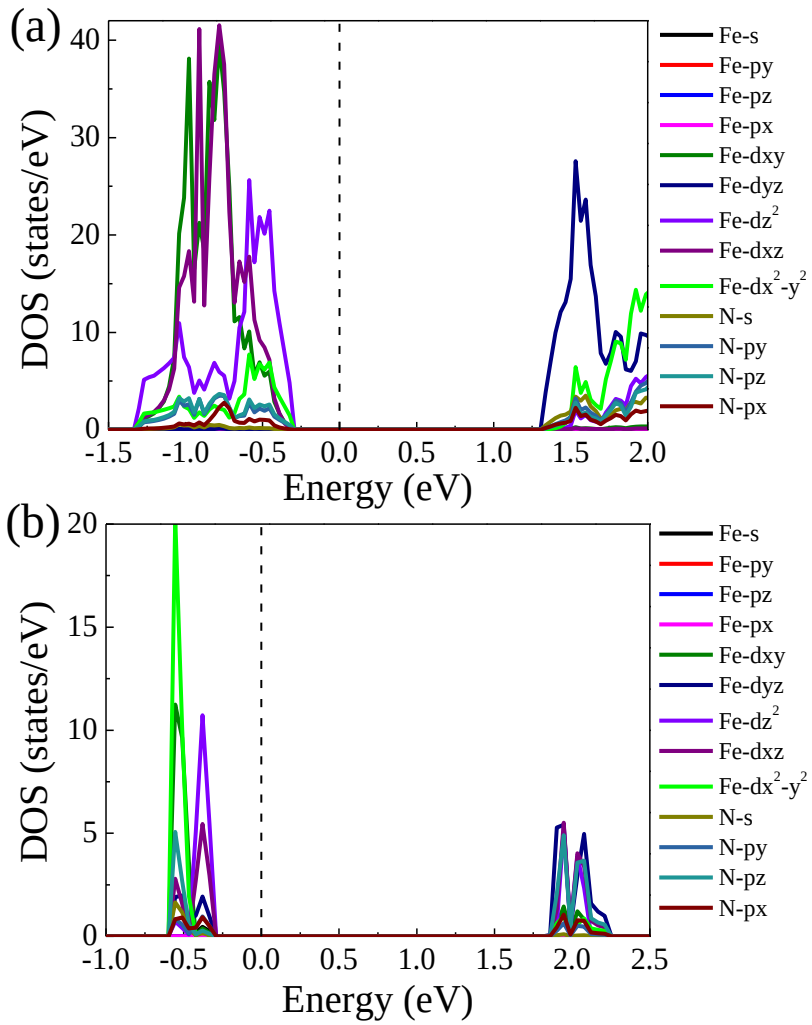

Figure S7: Partial density of states of *Fdd*2-FeN_{10} and *P*-1(No.1)-FeN_{10} at 0 GPa.

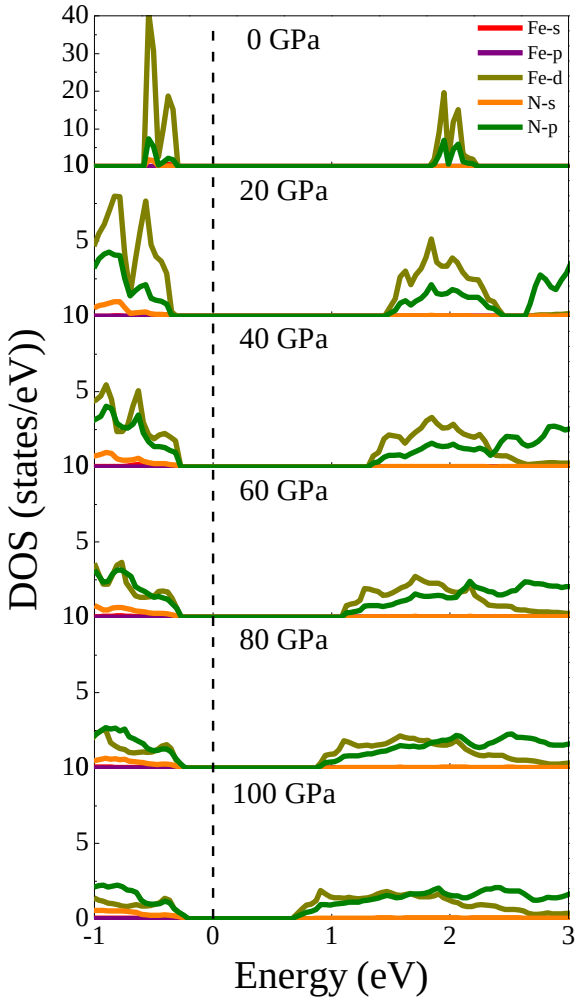

Figure S8: Partial density of states of *P*-1(No.1)-FeN_{10} at 0-100 GPa.

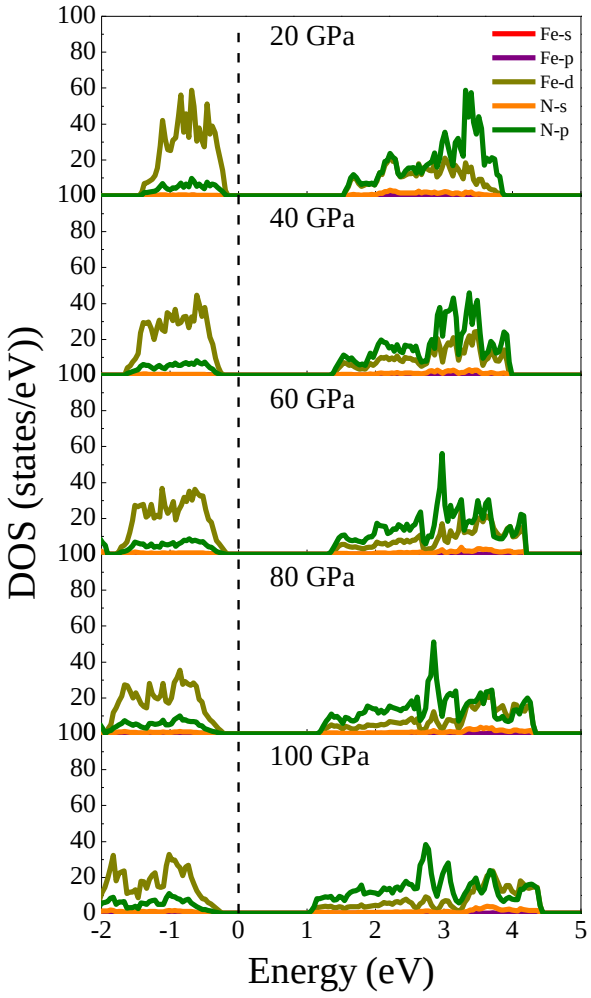

Figure S9: Partial density of states of *Fdd*2-FeN_{10} above 10 GPa.