Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Phase Diagram, Stability and Electronic Property of Fe-P System under High Pressure: a First-Principles study

Ziyuan Zhao[a], Lulu Liu[a], Shoutao Zhang[a], Tong Yu[a], Fei Li[a] and Guochun Yang[a,b,*]

a. Centre for Advanced Optoelectronic Functional Materials Research and Key Laboratory for UV Light-Emitting Materials and Technology of Ministry of Education, Northeast Normal University, Changchun 130024, China

b. State Key Laboratory of Superhard Materials, Jilin University, Changchun 130012, China

Email address: yanggc468@nenu.edu.cn

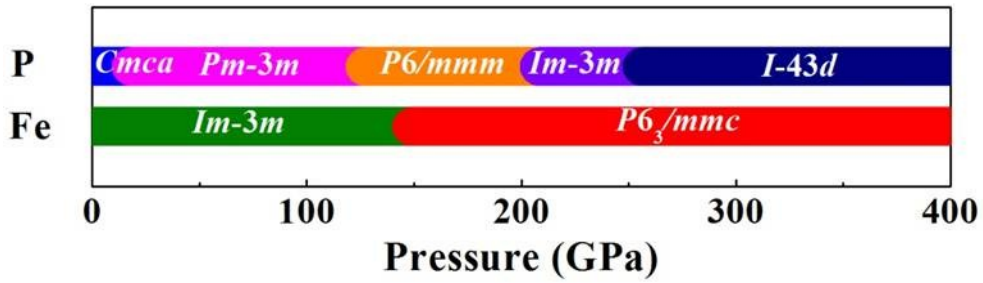

Figure S1. Pressure phase diagram of the elementary substances of Fe and P. The *bcc* phase (*Im*-3*m*) of element Fe is stable at ambient pressure until 149 GPa and the *hcp* structure ($P6_3/mmc$) is more stable at high pressure. For element P, the phase of space group *Cmca*, *Pm*-3*m*, *P*6/*mmm*, *Im*-3*m*, and *I*-43*d* are presented in range of 0 - 18 GPa, 18 - 127 GPa, 127 - 208 GPa, 208 - 256 GPa, and 256 - 400 GPa, respectively.

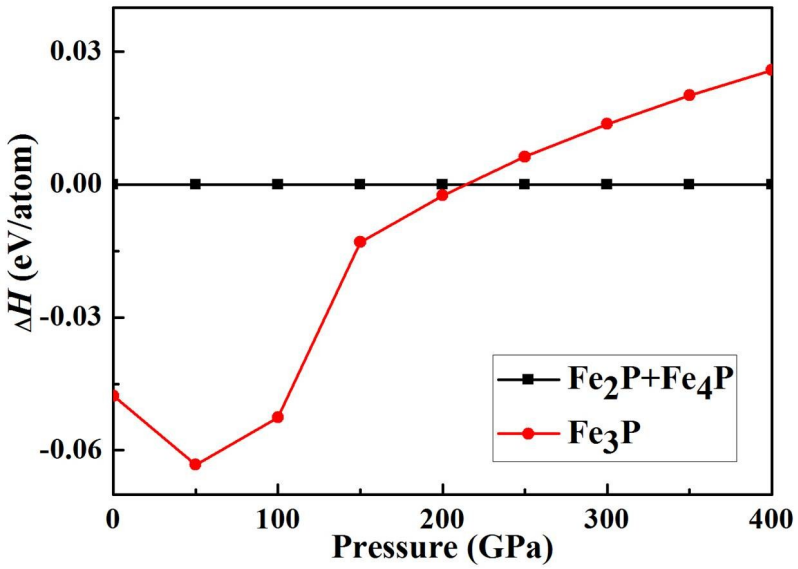

Figure S2. The calculated enthalpy difference as a function of pressure, for the reaction

equation: $2Fe_3P \leftrightarrow Fe_2P + Fe_4P$. $I\bar{4}$ and *Cmcm* referred to the symmetry of the Fe_3P phase, $P\bar{6}2m$ and *Pnma* referred to the symmetry of the Fe_2P phase, and $P2_13$ and $C2/c$ referred to the symmetry of the Fe_4P. This indicates that Fe_3P compound decomposes into Fe_2P and Fe_4P above 214 GPa.

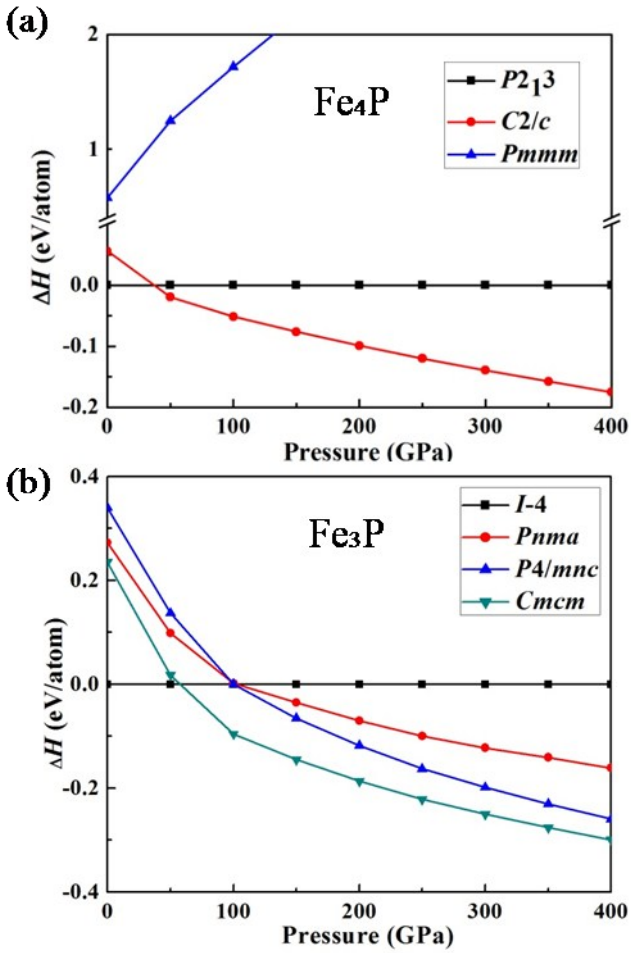

Figure S3. Enthalpy differences of Fe-P compounds as a function of pressure. (a) Fe_4P phase. (b) Fe_3P phase.

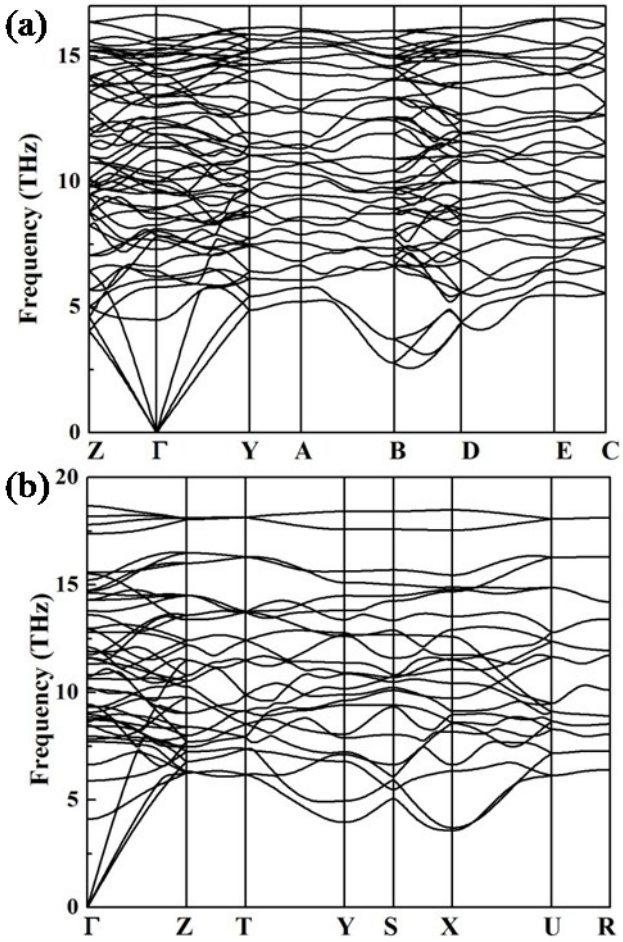

Figure S4. Calculated phonon spectra for Fe-P compounds at the respective stable pressure range. (a) The *C*2/*c*-structure Fe_4P at 100 GPa. (b) The *Cmcm*-structure Fe_3P at 100 GPa.

Table S1. Calculated integrated crystal orbital Hamiltonian populations (ICOHPs) of Fe-Fe, and Fe-P pairs in Fe_4P.

Phase	Pressure (GPa)	Atom	Atom	Distance (Å)	ICOHP(E_f)
Fe_4P-*C*2/*c*	200	**Fe1**	**P10**	**2.18037**	**-1.79724**
		Fe 4*s*	P 3*s*	2.18037	0.06782
		Fe 4*s*	P 3*p*	2.18037	0.00166
		Fe 3*p*	P 3*s*	2.18037	-0.13780
		Fe 3*p*	P 3*p*	2.18037	-0.45490
		Fe 3*d*	P 3*s*	2.18037	-0.19935
		Fe 3*d*	P 3*p*	2.18037	-1.07467

Fe5	**Fe8**	**2.17814**	**-4.97046**
Fe 4*s*	Fe 4*s*	2.17814	0.22743
Fe 4*s*	Fe 3*p*	2.17814	-0.54495
Fe 4*s*	Fe 3*d*	2.17814	-1.57096
Fe 3*p*	Fe 4*s*	2.17814	-0.11569
Fe 3*p*	Fe 3*p*	2.17814	-0.20230
Fe 3*p*	Fe 3*d*	2.17814	-0.70508
Fe 3*d*	Fe 4*s*	2.17814	-0.33689
Fe 3*d*	Fe 3*p*	2.17814	-0.84201
Fe 3*d*	Fe 3*d*	2.17814	-0.88004

Table S2. The Δ*H* values of the three Fe_3P phases (space group *Cmcm*, *P4/mnc* and *Pnma*) at 64 GPa.

Phase	**Enthalpy (eV/atom)**
Fe_3P-*Cmcm*	0.00
Fe_3P-*P*4/*mnc*	0.113
Fe_3P-*Pnma*	0.087