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Supplementary Information

A theoretical investigation on the structural stability, superconductivity, optical, and thermodynamic properties of Ir_2P under pressure

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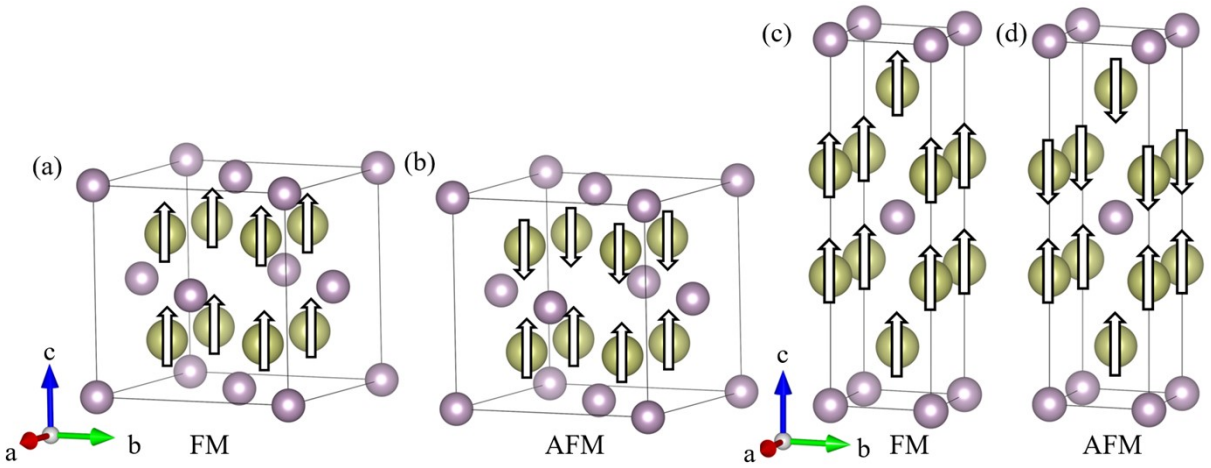

Fig. **S1** All possible magnetic configurations for the (a, b) $Fm\bar{3}m$ and (c, d) $I4/mmm$ phases of Ir_2P. The gold and purple spheres represent Ir and P atoms, respectively

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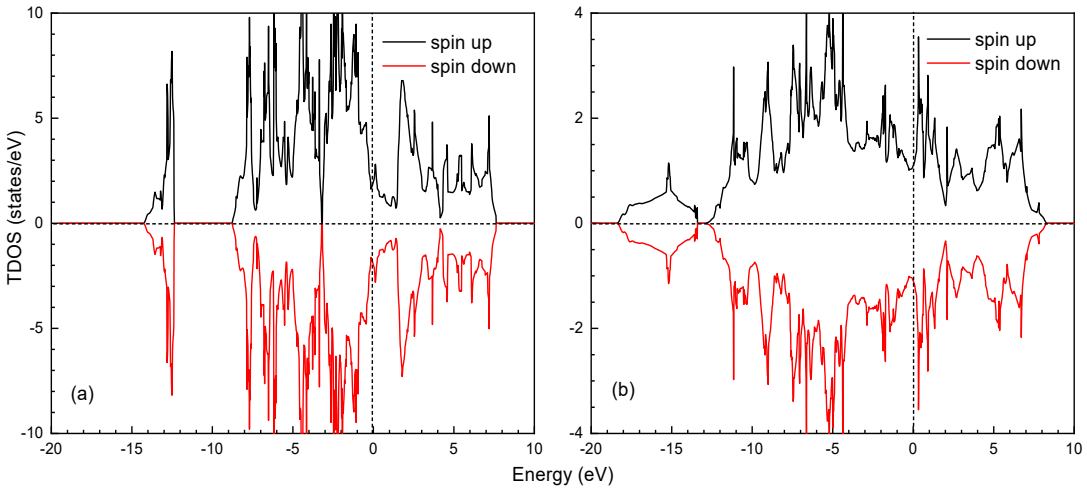

Fig. **S2**. Calculated spin-polarized density of states for the (a) $Fm\bar{3}m$ and (b) $I4/mmm$ phases of Ir_2P at 0 and 120 GPa, respectively

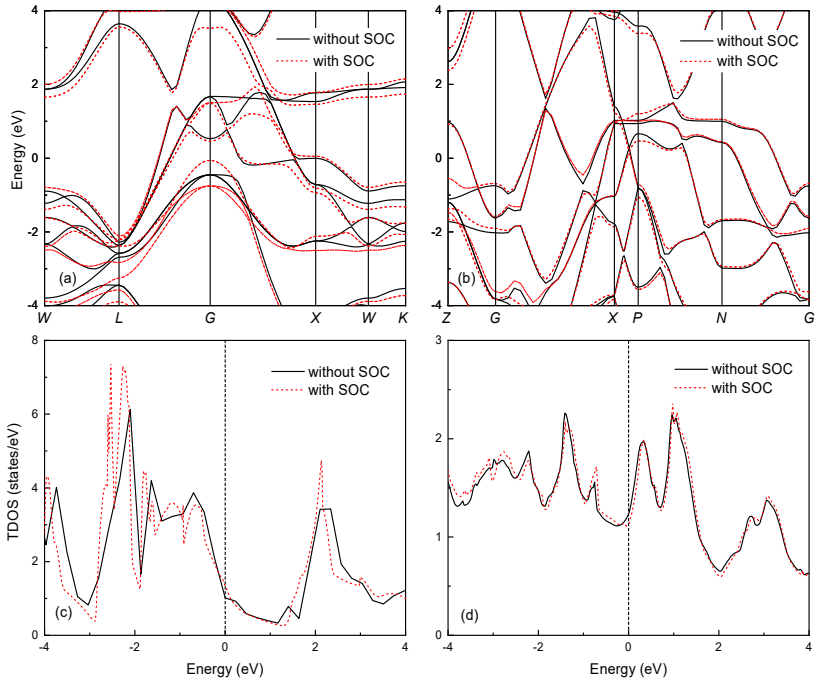

Fig. **S3** Band structures and density of states for the (a,c) $Fm\bar{3}m$ and (b,d) $I4/mmm$ phases of Ir_2P with and without spin-orbit effect at 0 and 120 GPa, respectively

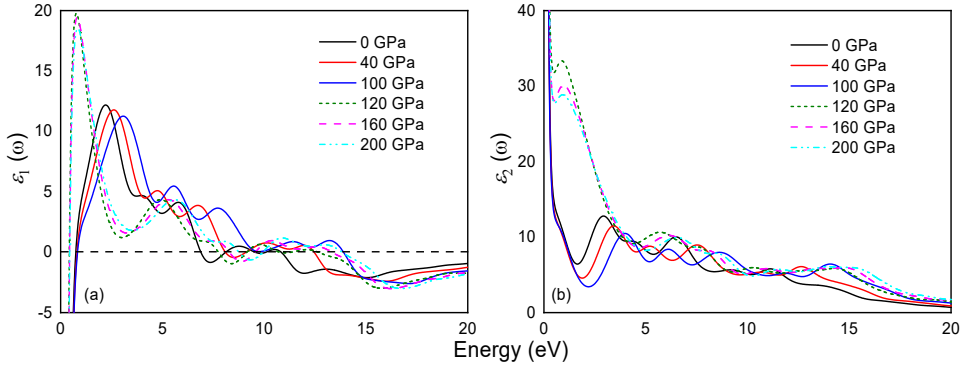

Fig. S4. Energy dependence of the (a) real part $\varepsilon_1(\omega)$ and (b) imaginary part $\varepsilon_2(\omega)$ of the complex dielectric function for the $Fm\bar{3}m$ and $I4/mmm$ phases of Ir_2P at different pressures. The solid and dashed lines represent the $Fm\bar{3}m$ and $I4/mmm$ phases, respectively.

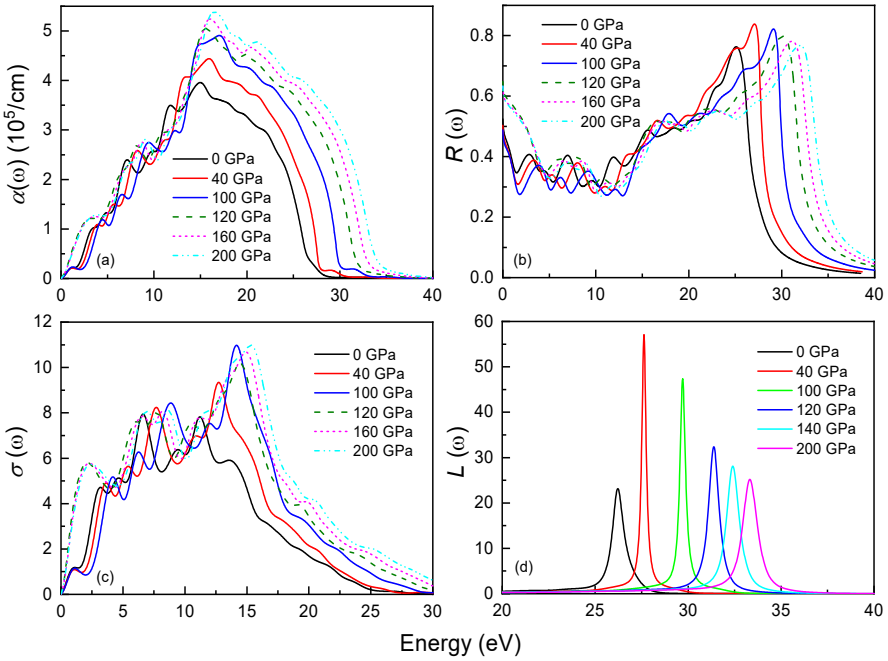

Fig. S5. Energy dependence of the (a) absorption coefficient $\alpha(\omega)$, (b) reflectance $R(\omega)$, (c) optical conductivity $\sigma(\omega)$, and (d) loss function $L(\omega)$ for the $Fm\bar{3}m$ and $I4/mmm$ phases of Ir_2P at different pressures. The solid and dashed lines represent the $Fm\bar{3}m$ and $I4/mmm$ phases, respectively.

Table **S1** The Bader charge analysis for Ir and P of $Fm\bar{3}m$ and $I4/mmm$ of Ir_2P

Space group	Pressure (GPa)	Atom	Number	Charge transfer (e)
$Fm\bar{3}m$	0	Ir	2	-0.21
		P	1	0.42
	100	Ir	2	-0.355
		P	1	0.71
	120	Ir	2	-0.265
		P	1	0.53
$I4/mmm$	200	Ir	2	-0.31
		P	1	0.62