Pressure induced multi-centre bonding and metal-insulator transition in $PtAl_2$

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SUPPLEMENTARY MATERIAL

Lindhard succeptibility: According to non-interacting Fermi gas model the Lindhard susceptibility function can be written as,

$$\chi_0(\vec{q},\omega) = \frac{2}{\hbar}\int d\vec{k} f_{\vec{k}}(1 - f_{\vec{k}'})\left[\frac{1}{\omega + (\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}'}) + i\eta} - \frac{1}{\omega - (\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}'}) + i\eta}\right]$$

Where, ε is the electron's eigenvalue, $k'=k+q$ and f is the Fermi-Dirac distribution function. After simplification the real and imaginary parts of this complex function can be written as,

$$Re[\chi_0(\vec{q},\omega)] = \frac{2}{(2\pi)^2}\int_{BZ} \frac{f_{\vec{k}'} - f_{\vec{k}}}{\omega + (\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}'})} d\vec{k}$$

$$Im[\chi_0(\vec{q},\omega)] = \frac{1}{2\pi}\int_{BZ} (f_{\vec{k}'} - f_{\vec{k}})\delta(\omega + \varepsilon_{\vec{k}} - \varepsilon_{\vec{k}'}) d\vec{k}$$

In the static limit ($\omega \to 0$) and $Im[\chi_0(\vec{q},\omega)] = 0$; using rescaled coordinates $q \to k/k_F$ (k_F is the Fermi wave vector), the Lindhard function in 1, 2 and 3 dimension can be written as,

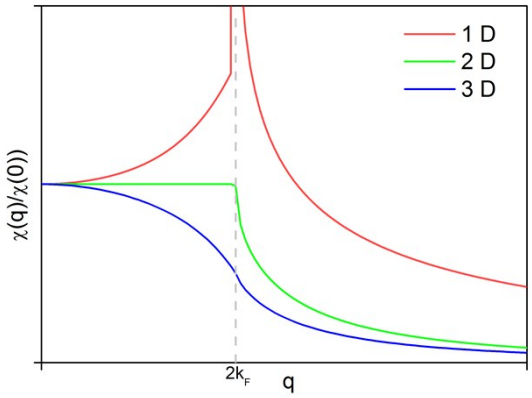
$$Re\ \chi_0 \propto -\frac{1}{2q} ln\left|\frac{1 + q/2}{1 - q/2}\right| \quad \text{for 1D}$$

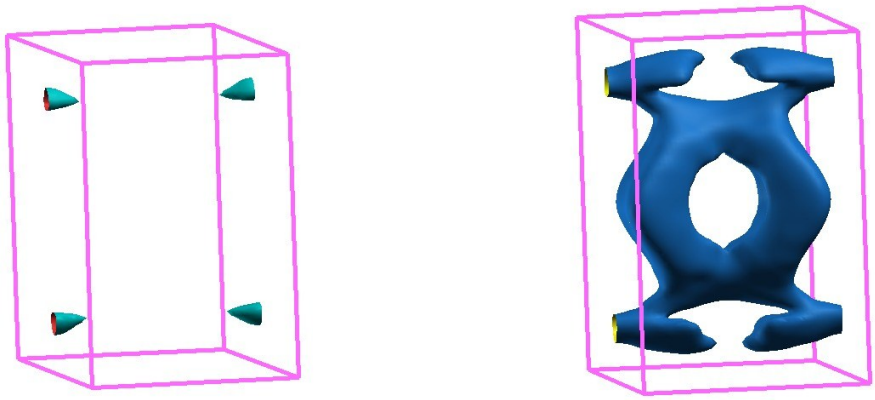
$$Re\ \chi_0 \propto \begin{cases} -1/E_F, & q < 2k_F \\ -\left(1 - \sqrt{1 - (2/q)^2}\right), & q \geq 2k_F \end{cases} \quad \text{for 2D}$$

and

$$Re\ \chi_0 \propto -\left[1 + \frac{1 - (q/2)^2}{q} ln\left|\frac{1 + q/2}{1 - q/2}\right|\right] \quad \text{for 3D}$$

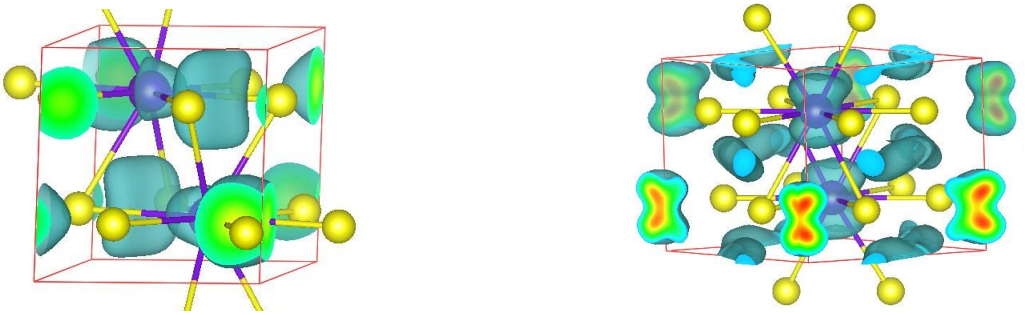
The graphical representation of $\chi(q)$ for different dimension is shown below. Hence, the electronic response function diverges at $q=2k_F$ for 1D systems and is discontinuous at $q=2k_F$ for 2D systems. Our system is quasi 2D perpendicular to **b**-crystallographic axis.





(a) (b)

FIG. S1: Fermi surfaces for other two bands near 28 GPa in orthorhombic Pnma structure, horizontal direction is $\mathbf{k_z}$, vertical direction is $\mathbf{k_x}$ and $\mathbf{k_y}$ is perpendicular downward to the plane of paper.



(a) (b)

FIG. S2: Band decomposed charge density isosurface for isovalue 0.06, (a) corresponds to top of the valence band near Z-point (b) corresponds to bottom of the conduction band near S-point. All the charge density computed within an energy window of ±0.1 eV. Yellow (small) sphere represents Al-atoms and Violet (big) sphere represents Pt-atoms.

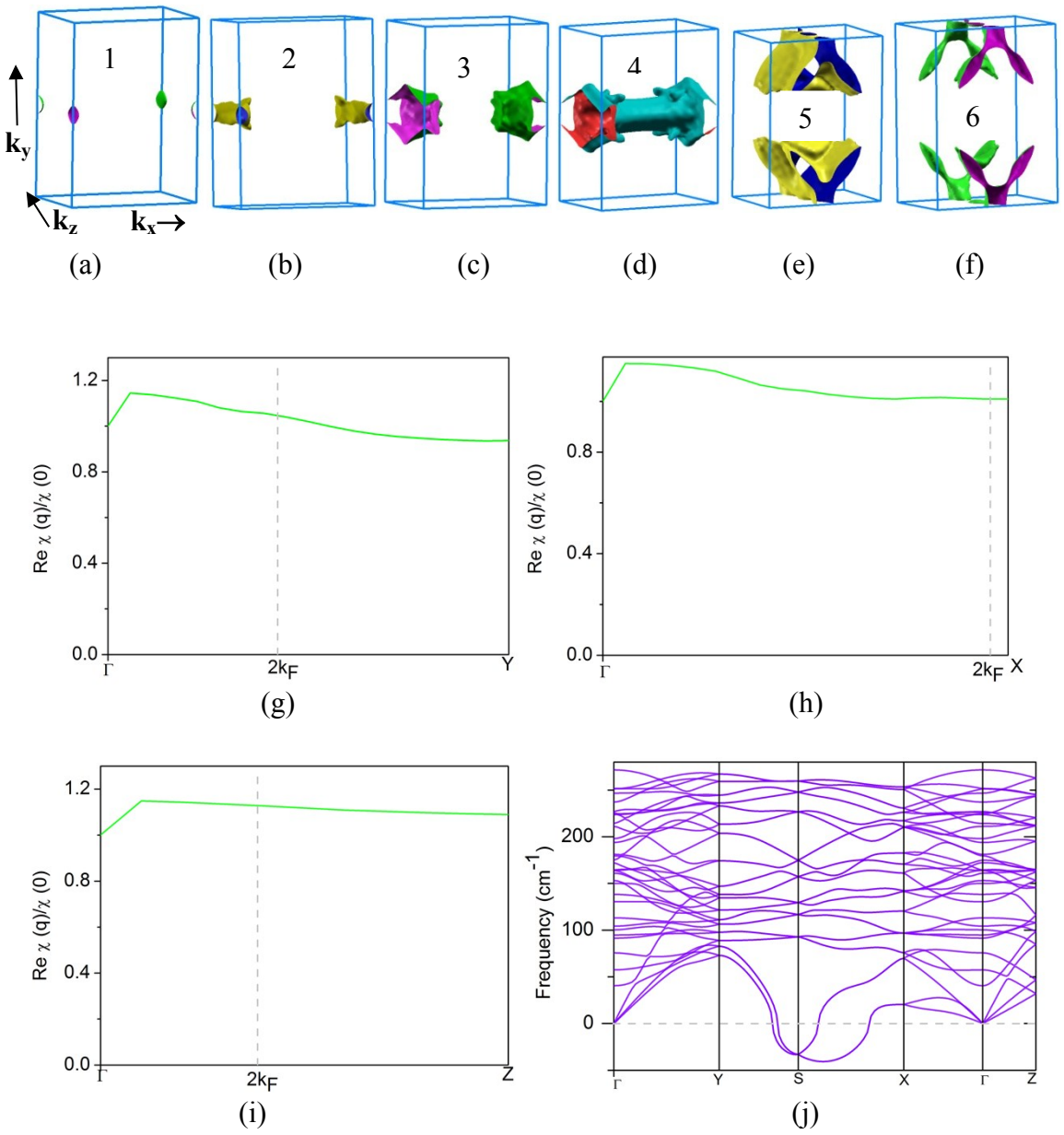


FIG. S3: Fermi surface (FS), electronic susceptibility and phonons of $PtIn_2$ in the Pnma phase near Pnma to C2/m transition. (a-f) Fermi sheets corresponding to different bands, (g-i) electronic susceptibility along different high symmetry direction of BZ, and (j) phonon dispersions along some high symmetry directions of BZ.