tight binding fit of β-(ET)2AuCl2

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The Hamiltonian is

$$H = \begin{pmatrix} t_c \exp(ik_z c) + t_c \exp(-ik_z c) & , & t_{a1} \exp(-ik_x a) + t_p \exp(i(k_x a + k_z c)) \\ & & +t_{a2} + t_q \exp(ik_z c) \\ * & , & t_c \exp(ik_z c) + t_c \exp(-ik_z c) \end{pmatrix} \quad (1)$$

$$+ \begin{pmatrix} 0 & , & t_{a2c} \exp(i(-k_x a - k_y b - k_z c)) + t_{qc} \exp(i(-k_x a - k_y b)) \\ * & , & 0 \end{pmatrix}. \quad (2)$$

(1) is the contribution inside the layer. (2) comes from interlayer. The intralayer contribution is on the order of 0.1 eV, while the interlayer one is on the order of 0.01eV.

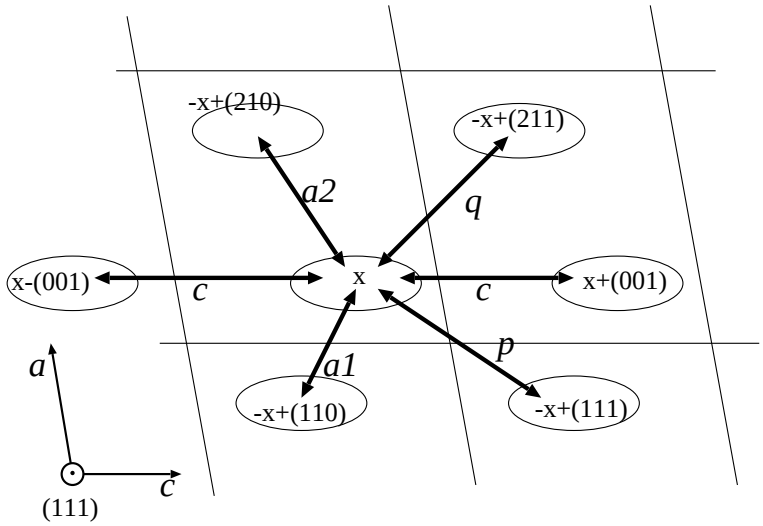

Figure 1: A schematic crystal structure. The molecules on the layer above this one locates at $X + (111)$. file=/home/kino/work/ET-AuCl2/tex/crystal1.obj

P	a1 a2c	a2 qc	p	q	c
0	-0.181199998 6.53999997e-03	-9.38000008e-02 2.51999986e-03	-4.56000008e-02	2.90000010e-02	-2.66000014e-02
4	-0.262600005 1.47159994e-02	-0.146200016 1.11680012e-02	-9.72000137e-02	7.18000010e-02	-3.07999998e-02
8	-0.363509446 2.15497315e-02	-0.172976032 1.21034654e-02	-0.179449081	0.114870518	-6.60938546e-02
12	-0.389709532 2.09897365e-02	-0.186986014 1.68634672e-02	-0.227399155	0.142890483	-7.87238628e-02
16	-0.388709515 2.43253391e-02	-0.187646016 2.08542701e-02	-0.243759155	0.157110482	-7.64938667e-02
20	-0.401589572 3.06089427e-02	-0.191805974 1.79434735e-02	-0.257559150	0.188470498	-6.43338710e-02

Table 1: fitted parameters, a2c=a parameter to the molecule at a2-(111), qc= to the molecule at q-(111). file=/home/kino/work/ET-AuCl2/3Dfit.dat

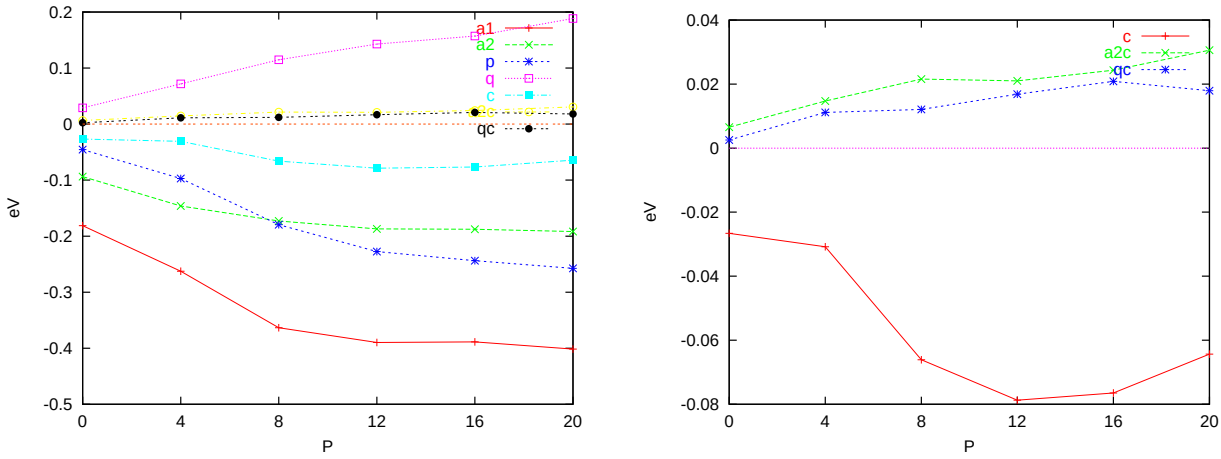

Figure 2: fitted parameters, file=/home/kino/work/ET-AuCl2/plot.gnu

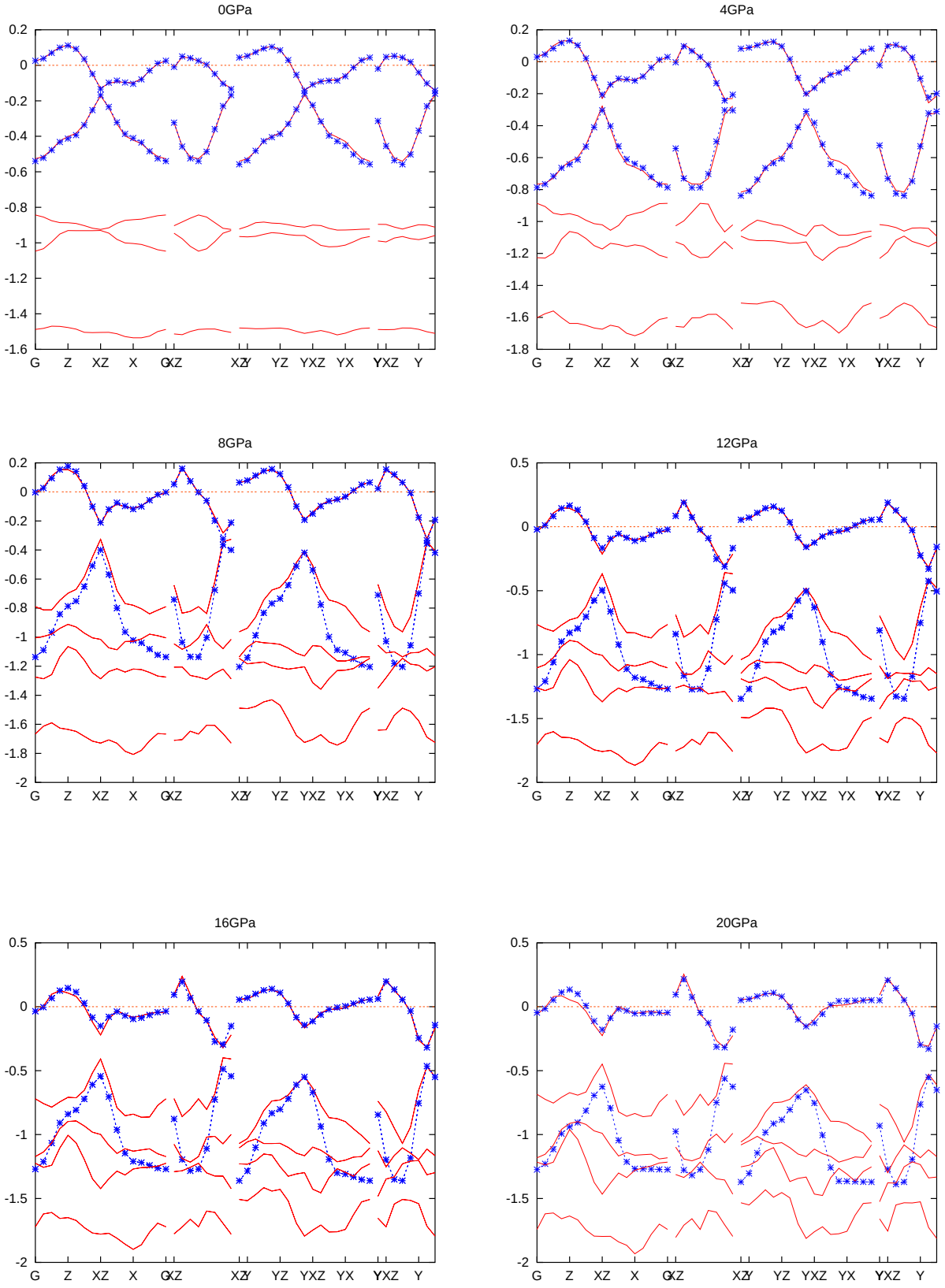

Figure 3: The Miyazaki's results (red) and their TB fit (blue) at k_y=0 and k_y=π. The HOMO-1 band equal to and more than 8 GPa mixes with other bands. Therefore the fitting is not good for the HOMO-1 band. In reality, the wavefunction of the HOMO-3 at Γ point is made of the same BEDT-TTF molecular orbital as the HOMO. file=tbfit.??GPa.true3D/