tight binding fit of β'-(ET)2ICl2

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The Hamiltonian is

$$H = \begin{pmatrix} t_c \exp(ik_z c) + t_c \exp(-ik_z c) & , & t_{p1} \exp(ik_z c) + t_{p2} \exp(-ik_y b) \\ & & +t_{q2} + t_{q1} \exp(i(k_y b + kzc)) \\ * & , & t_c \exp(ik_z c) + t_c \exp(-ik_z c) \end{pmatrix} \quad (1)$$

$$+ \begin{pmatrix} 0 & , & t_{p2c} \exp(i(k_x a + k_z c)) + t_{q1c} \exp(i(k_x a + 2k_z c)) \\ * & , & 0 \end{pmatrix}. \quad (2)$$

(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 about 0.005eV.

P	p1	p2	q1	q2	c
	e0	p1c	q2c		
0	-0.206404	0.027600	-0.101198	-0.055354	-0.029396
	-0.232396	-0.000032	0.004762		
4	-0.278676	0.065686	-0.153058	-0.098368	-0.029016
	-0.330402	-0.000715	0.005614		
8	-0.325200	0.098200	-0.176800	-0.116600	-0.040000
	-0.381600	-0.002472	0.004400		
12	-0.334160	0.139680	-0.190000	-0.140160	-0.041400
	-0.412960	-0.007444	0.002232		

Table 1: fitted parameters, p1c=a parameter to the molecule at p1+(111), q2c= to the molecule at q2+(111). file=/home/kino/work/ET-ICl2/3Dfit.dat. convert=awk -f fit2tex.awk 3Dfit.dat

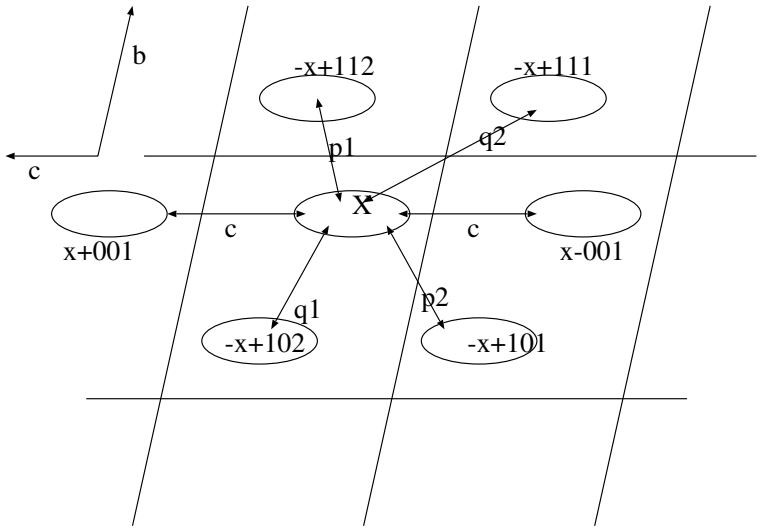

Figure 1: A schematic crystal structure. The molecules on the layer above this one locates at $X + (111)$. file=/home/kino/work/ET-ICl2/tex/crystal1.obj

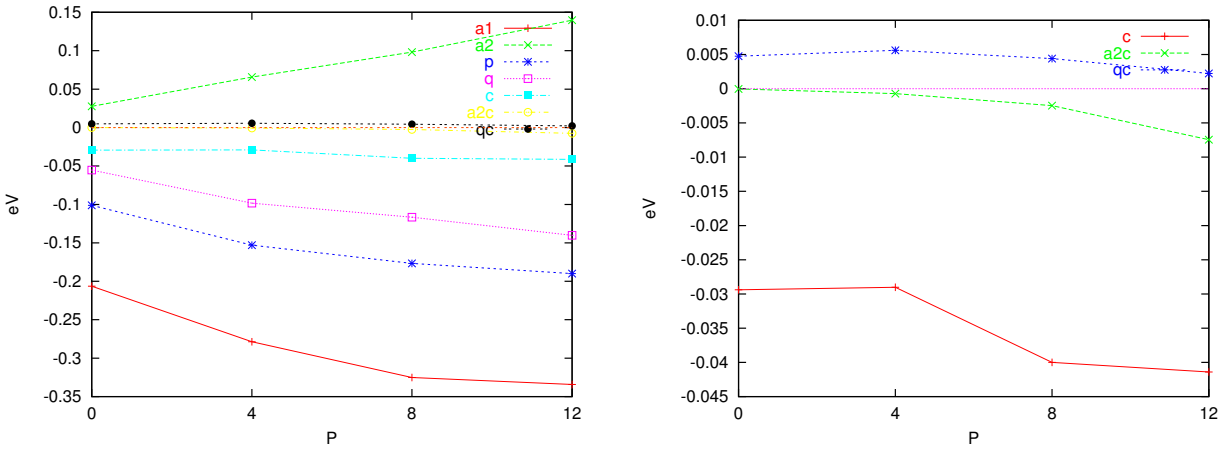

Figure 2: fitted parameters, file=/home/kino/work/ET-ICl2/plot.gnu

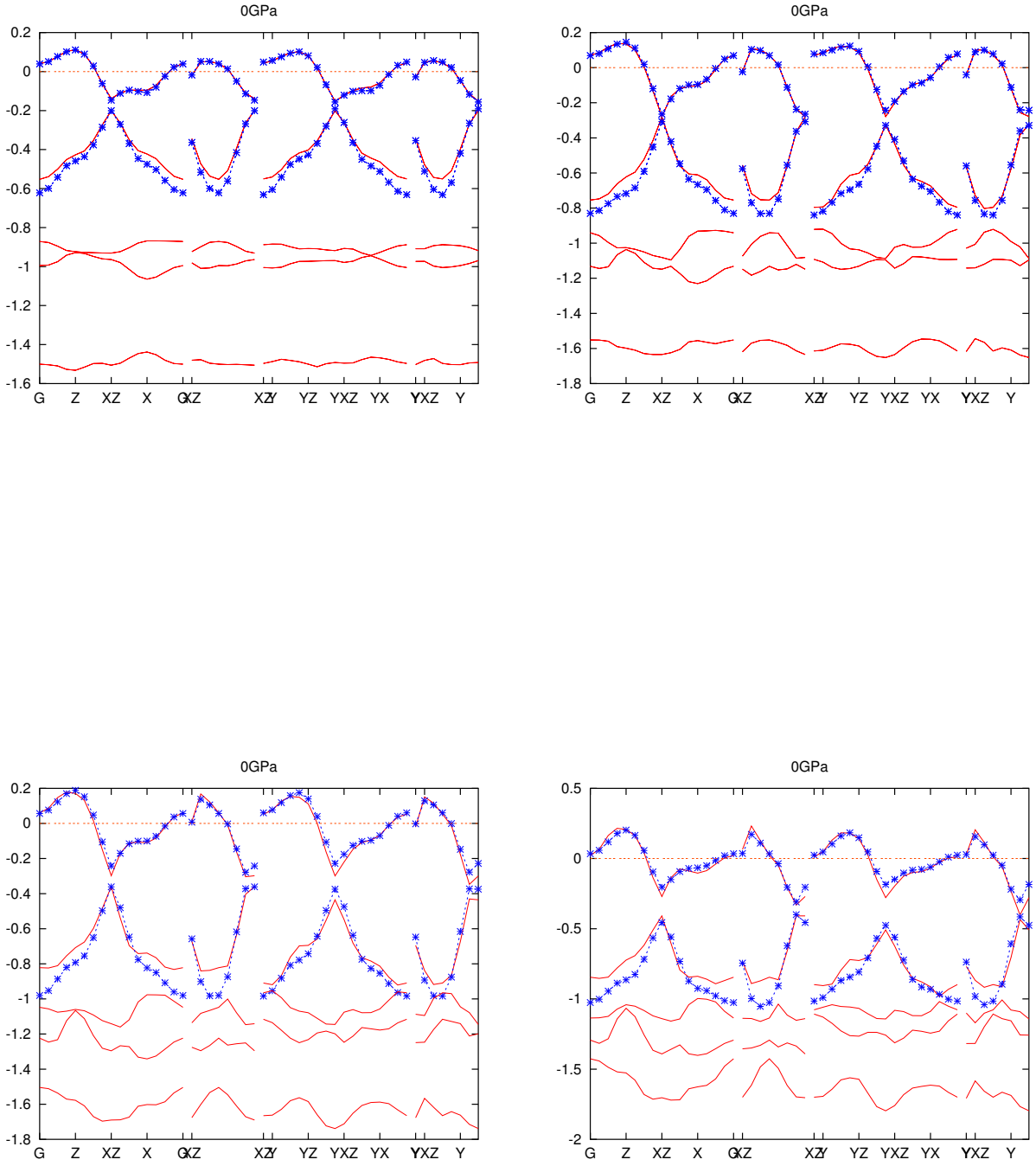

Figure 3: The Miyazaki's results (red) and their 3TB fit (blue) at k_x=0 and k_x=π. file=SCF?.3D/