NOTE
basis : $g_1 = px$, $g_2 = py$, $g_3 = pz$, $g_4 = dxy$, $g_5 = dyz$, $g_6 = dzx$.

$$H(k) = \begin{bmatrix} H_{x,x} & 0 & 0 & H_{x,xy} & 0 & H_{x,zx} \\ & H_{y,y} & 0 & H_{y,xy} & H_{y,yz} & 0 \\ & & H_{z,z} & 0 & H_{pz,dyz} & H_{z,zx} \\ & & & H_{xy,xy} & 0 & 0 \\ & & \dagger & & H_{yz,yz} & 0 \\ & & & & & H_{zx,zx} \end{bmatrix}$$

$$H_{x,x} = E_p + 2cosk_x aV_{pp\sigma} + 2cosk_y aV_{pp\pi} + 2cosk_z aV_{pp\pi}$$

$$H_{x,xy} = 2isink_y aV_{pd\pi}$$

$$H_{x,zx} = 2isink_z aV_{pd\pi}$$

$$H_{y,y} = E_p + 2cosk_x aV_{pp\pi} + 2cosk_y aV_{pp\sigma} + 2cosk_z aV_{pp\pi}$$

$$H_{y,xy} = 2isink_x aV_{pd\pi}$$

$$H_{y,yz} = 2isink_z aV_{pd\pi}$$

$$H_{z,z} = E_p + 2cosk_x aV_{pp\pi} + 2cosk_y aV_{pp\pi} + 2cosk_z aV_{pp\sigma}$$

$$H_{z,yz} = 2isink_y aV_{pd\pi}$$

$$H_{z,zx} = 2isink_x aV_{pd\pi}$$

$$H_{xy,xy} = E_d + 2cosk_x aV_{dd\pi} + 2cosk_y aV_{dd\pi} + 2cosk_z aV_{dd\delta}$$

$$H_{yz,yz} = E_d + 2cosk_x aV_{dd\delta} + 2cosk_y aV_{dd\pi} + 2cosk_z aV_{dd\pi}$$

$$H_{zx,zx} = E_d + 2cosk_x aV_{dd\pi} + 2cosk_y aV_{dd\delta} + 2cosk_z aV_{dd\pi}$$

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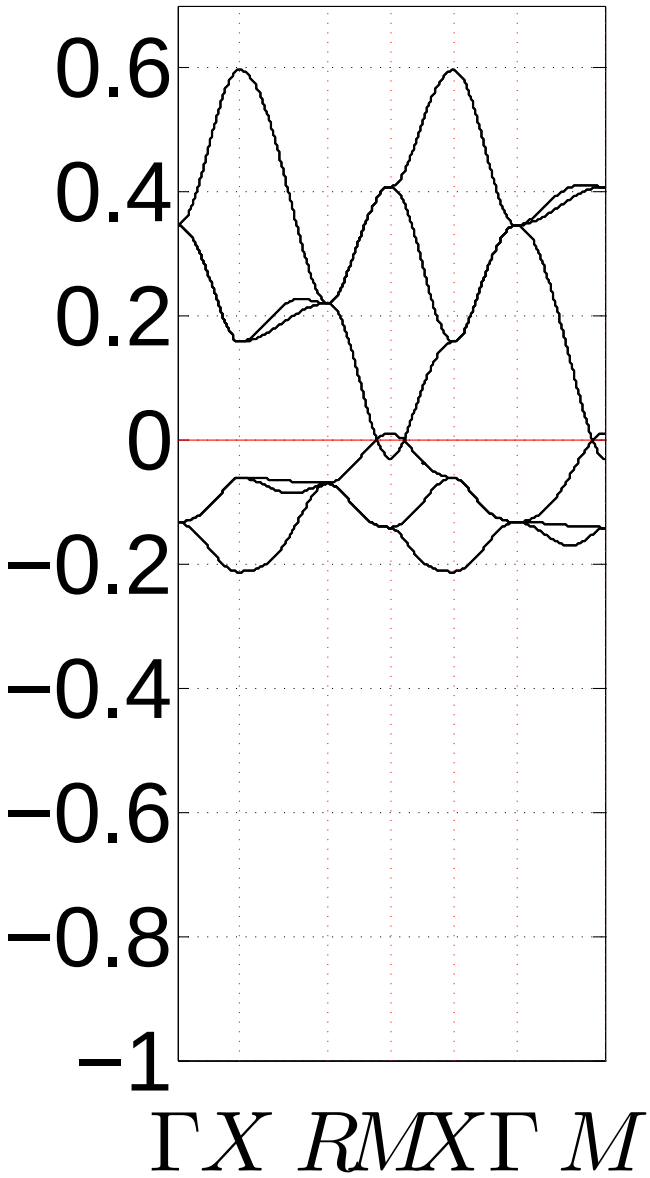

Figure 1: TB band with paras: $E_d = 0.28281$, $E_p = -0.10147$, $V_{pp\sigma} = 0.02005$, $V_{pp\pi} = -0.017848$, $V_{pd\pi} = 0.034711$, $V_{dd\pi} = 0.04694$, $V_{dd\delta} = -0.062523$