

TB Model

Hamiltonian non-zero Matrix Elements

$$H_{g_{xy}(x^2-y^2), g_{xy}(x^2-y^2)} = 2\cos(\vec{k}\vec{a}_x)V_{ggp} \\ + 2\cos(\vec{k}\vec{a}_y)V_{ggp} + 2\cos(\vec{k}\vec{a}_z)V_{ggd} + E_g$$

$$H_{g_{yz}(y^2-z^2), g_{yz}(y^2-z^2)} = 2\cos(\vec{k}\vec{a}_y)V_{ggp} \\ + 2\cos(\vec{k}\vec{a}_z)V_{ggp} + 2\cos(\vec{k}\vec{a}_x)V_{ggd} + E_g$$

$$H_{g_{zx}(z^2-x^2), g_{zx}(z^2-x^2)} = 2\cos(\vec{k}\vec{a}_z)V_{ggp} \\ + 2\cos(\vec{k}\vec{a}_x)V_{ggp} + 2\cos(\vec{k}\vec{a}_y)V_{ggd} + E_g$$

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$$\begin{aligned} H_{f_{x(y^2-z^2)}, f_{x(y^2-z^2)}} = & 2\cos(\vec{k}\vec{a}_x)V_{ffp} + 2\cos(\vec{k}\vec{a}_x)V_{ffp} \\ -2\cos(\vec{k}\vec{a}_y)V_{ffp} - 2\cos(\vec{k}\vec{a}_y)V_{ffd} & \\ -2\cos(\vec{k}\vec{a}_z)V_{ffp} - 2\cos(\vec{k}\vec{a}_z)V_{ffd} & \\ +E_f & \end{aligned}$$
$$\begin{aligned} H_{f_{y(z^2-x^2)}, f_{y(z^2-x^2)}} = & -2\cos(\vec{k}\vec{a}_x)V_{ffp} - 2\cos(\vec{k}\vec{a}_x)V_{ffd} \\ +2\cos(\vec{k}\vec{a}_y)V_{ffp} + 2\cos(\vec{k}\vec{a}_y)V_{ffp} & \\ -2\cos(\vec{k}\vec{a}_z)V_{ffp} - 2\cos(\vec{k}\vec{a}_z)V_{ffd} & \\ +E_f & \end{aligned}$$

$$\begin{aligned} H_{f_{z(x^2-y^2)}, f_{z(x^2-y^2)}} = & -2\cos(\vec{k}\vec{a}_x)V_{ffp} - 2\cos(\vec{k}\vec{a}_x)V_{ffd} \\ -2\cos(\vec{k}\vec{a}_y)V_{ffp} - 2\cos(\vec{k}\vec{a}_y)V_{ffd} & \\ +2\cos(\vec{k}\vec{a}_z)V_{ffp} + 2\cos(\vec{k}\vec{a}_z)V_{ffp} & \\ +E_f & \end{aligned}$$

TB Model

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$$H_{g_{xy}(x^2-y^2), f_{x(y^2-z^2)}} = i * 2\sin(\vec{k}\vec{a}_y)V_{fgp} + i * 2\sin(\vec{k}\vec{a}_y)V_{fgd}$$

$$H_{g_{xy}(x^2-y^2), f_{y(z^2-x^2)}} = i * 2\sin(\vec{k}\vec{a}_x)V_{fgp} + i * 2\sin(\vec{k}\vec{a}_x)V_{fgd}$$

$$H_{g_{yz}(y^2-z^2), f_{y(z^2-x^2)}} = i * 2\sin(\vec{k}\vec{a}_z)V_{fgp} + i * 2\sin(\vec{k}\vec{a}_z)V_{fgd}$$

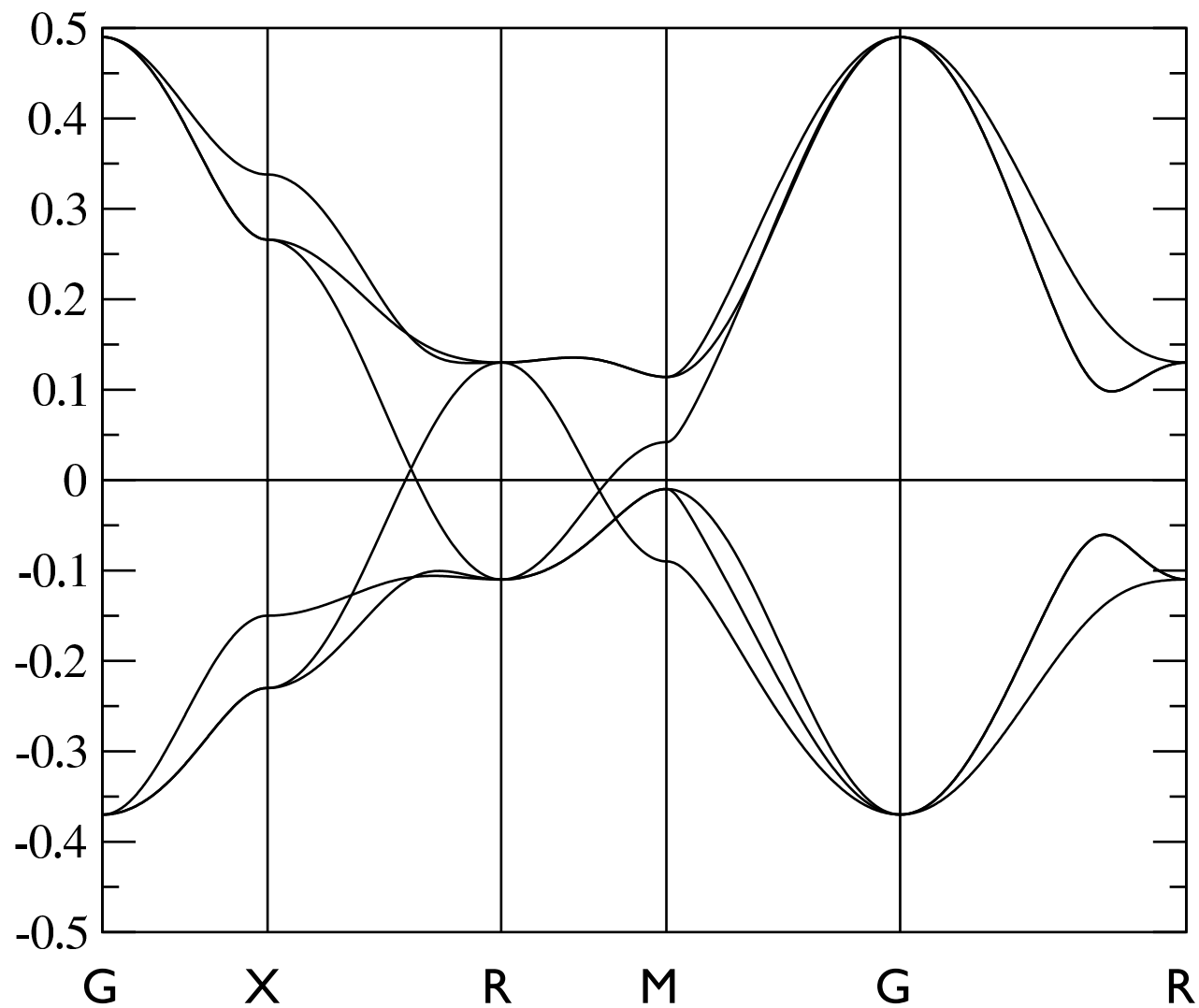
$$H_{g_{yz}(y^2-z^2), f_{z(x^2-y^2)}} = i * 2\sin(\vec{k}\vec{a}_y)V_{fgp} + i * 2\sin(\vec{k}\vec{a}_y)V_{fgd}$$

$$H_{g_{zx}(z^2-x^2), f_{x(y^2-z^2)}} = i * 2\sin(\vec{k}\vec{a}_z)V_{fgp} + i * 2\sin(\vec{k}\vec{a}_z)V_{fgd}$$

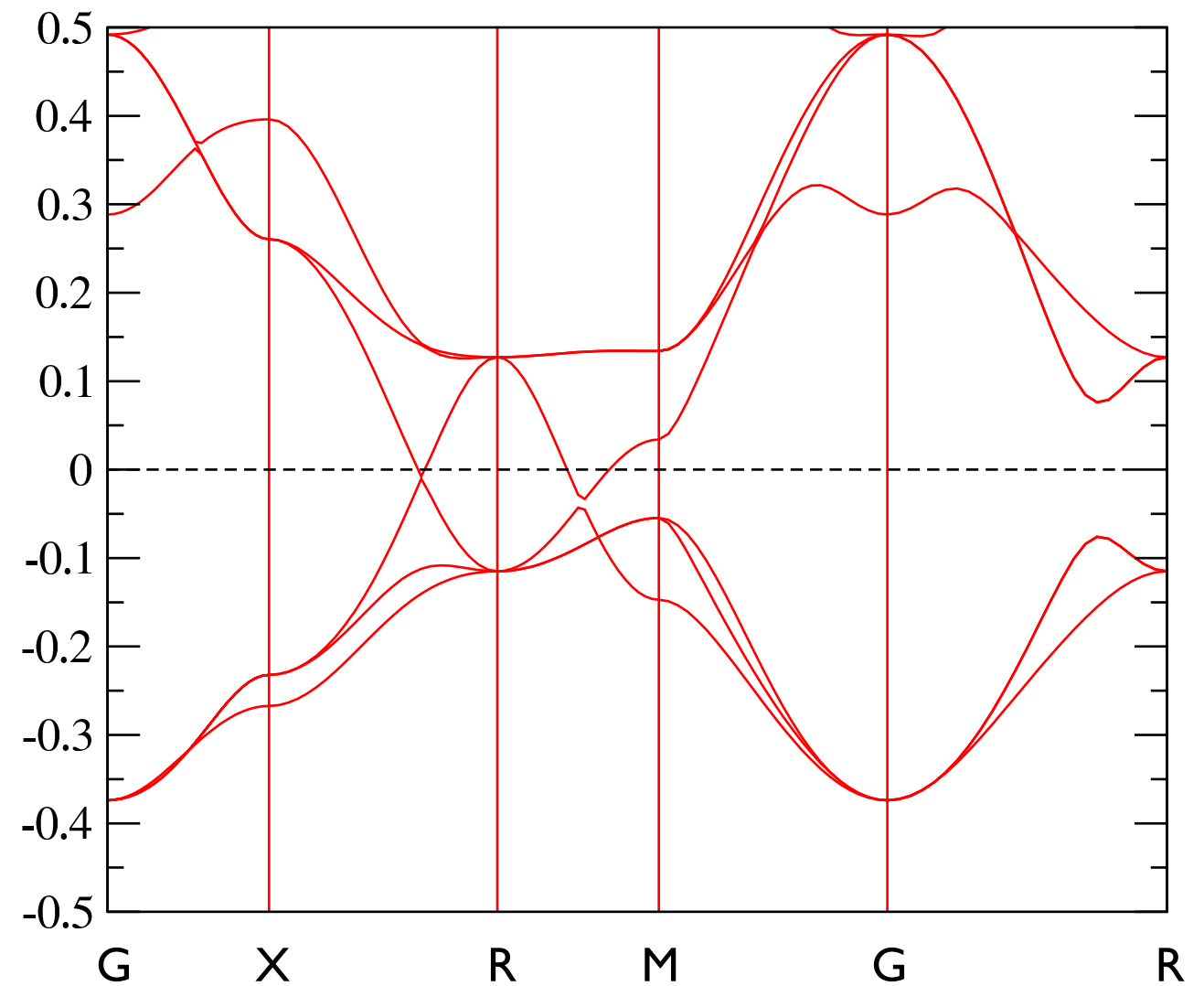
$$H_{g_{zx}(z^2-x^2), f_{z(x^2-y^2)}} = i * 2\sin(\vec{k}\vec{a}_x)V_{fgp} + i * 2\sin(\vec{k}\vec{a}_x)V_{fgd}$$

Best fitting

TB



ab-initio



$E_g = -0.12$;
 $E_f = 0.19$;
 $V_{ffp} = +0.019$; $V_{ffd} = -0.075$;
 $V_{fgp} = 0.05$; $V_{fgd} = 0.00$;
 $V_{ggp} = -0.035$; $V_{ggd} = -0.055$;