

Higher-order Weyl Semimetals

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where $\gamma_{x,y}$ represent the intra-cell coupling along x,y , $\{\Gamma_\alpha\}$ are direct products of Pauli matrices, σ_i, κ_i , following $\Gamma_0 = \sigma^3 \kappa^0$, $\Gamma_i = -\sigma^2 \kappa^i$ for $i = 1, 2, 3$, and $\Gamma_4 = \sigma^1 \kappa^0$.

$$\Gamma_1 = \begin{pmatrix} & & i \\ & i & \\ -i & -i & \end{pmatrix}$$

$$\Gamma_3 = \begin{pmatrix} & & 1 \\ & i & \\ -i & & -i \\ & i & \end{pmatrix}$$

$$\Gamma_2 = \begin{pmatrix} & & 1 \\ & -1 & \\ & -1 & \\ 1 & & \end{pmatrix}$$

$$\Gamma_4 = \begin{pmatrix} & & 1 \\ & & \\ 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}$$

$$\Gamma_1 \Gamma_3 = \begin{pmatrix} & -1 & \\ 1 & & \\ & 1 & -1 \end{pmatrix}$$

Model and Formalism.– We start with a simple model for HODSMs using spinless fermions from Ref. 38, whose Bloch Hamiltonian can be written as:

$$\begin{aligned}
 H_{HODSM}(\mathbf{k}) = & \left(\gamma_x + \frac{1}{2} \cos k_z + \cos k_x \right) \Gamma_4 + \sin k_x \Gamma_3 \\
 & + \left(\gamma_y + \frac{1}{2} \cos k_z + \cos k_y \right) \Gamma_2 + \sin k_y \Gamma_1,
 \end{aligned}
 \tag{1}$$

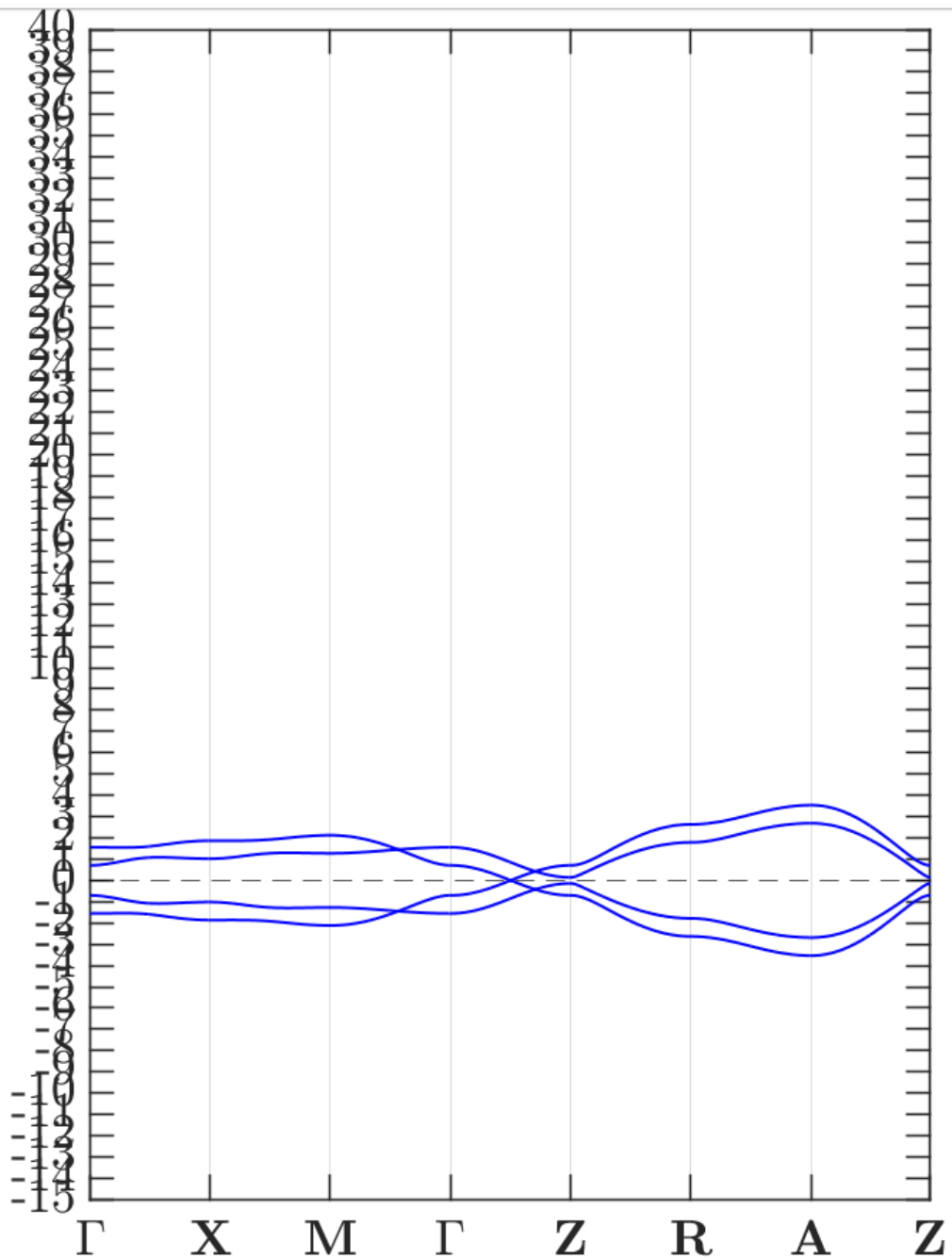
shown in Fig. 1(c-e). We first consider $H^1 = H_{HODSM} + m_1 i \Gamma_1 \Gamma_3$, which breaks time-reversal symmetry $\mathcal{T}, \mathcal{M}_x$,

$$\gamma_x = \gamma_y = \gamma.$$

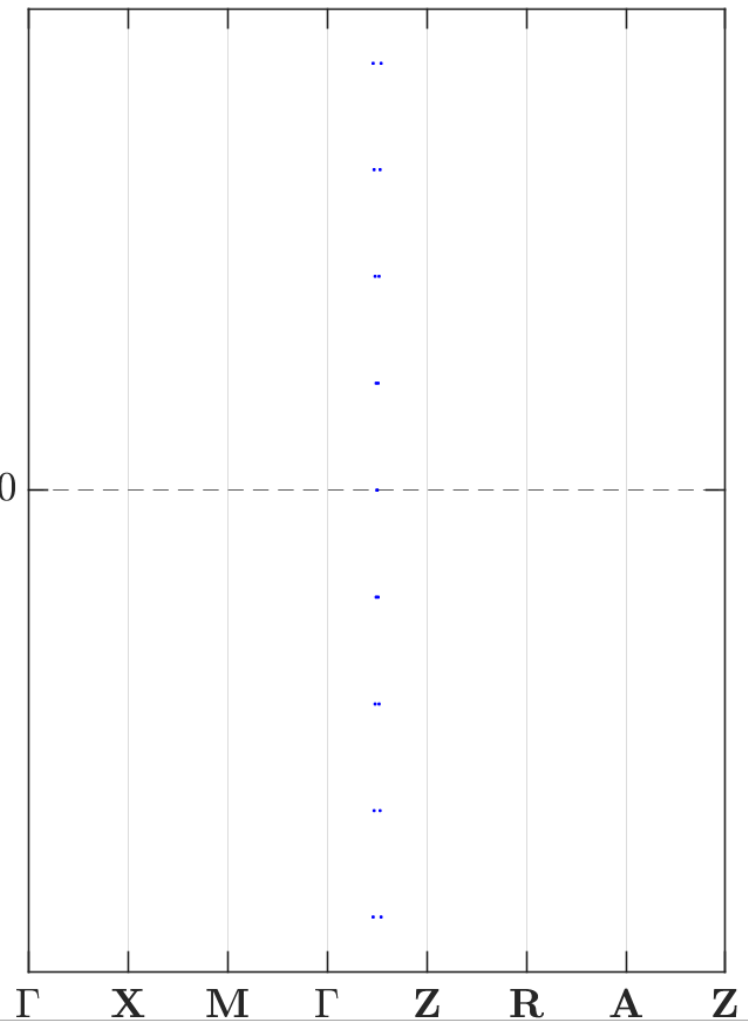
$$H = \begin{pmatrix} & & & -im_1 \\ & im_1 & & \\ & & \left(\gamma + \frac{1}{2} \cos(k_z) + \cos(k_x) \right) - i * \sin(k_x) & - \left(\gamma + \frac{1}{2} \cos(k_z) + \cos(k_y) \right) - i * \sin(k_y) \\ \left(\gamma + \frac{1}{2} \cos(k_z) + \cos(k_y) \right) - i * \sin(k_y) & \left(\gamma + \frac{1}{2} \cos(k_z) + \cos(k_x) \right) + i * \sin(k_x) & & \end{pmatrix}$$

$$\begin{pmatrix} \left(\gamma + \frac{1}{2} \cos(k_z) + \cos(k_x) \right) + i * \sin(k_x) & \left(\gamma + \frac{1}{2} \cos(k_z) + \cos(k_y) \right) + i * \sin(k_y) \\ - \left(\gamma + \frac{1}{2} \cos(k_z) + \cos(k_y) \right) + i * \sin(k_y) & \left(\gamma + \frac{1}{2} \cos(k_z) + \cos(k_x) \right) - i * \sin(k_x) \end{pmatrix}$$

Energy (eV)



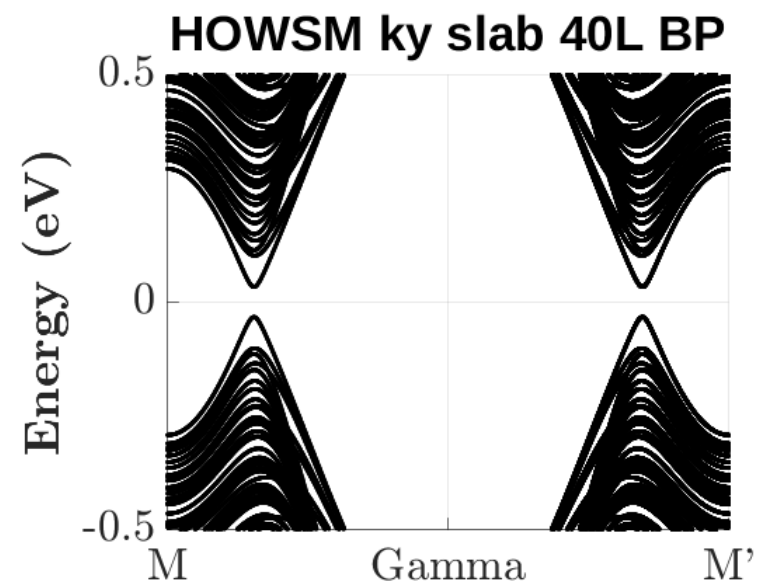
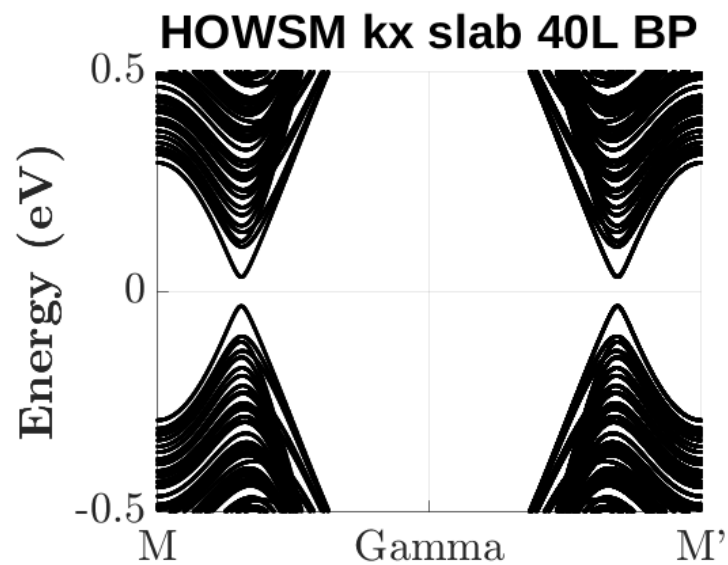
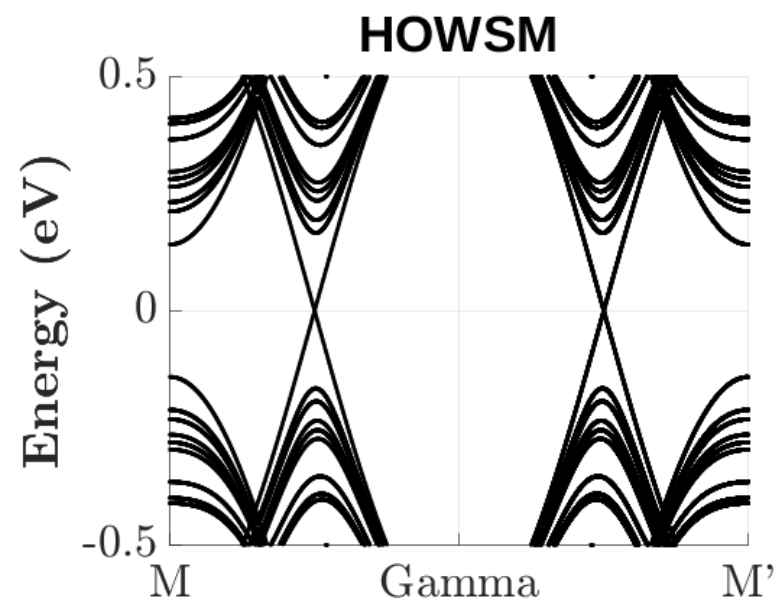
Energy (eV)



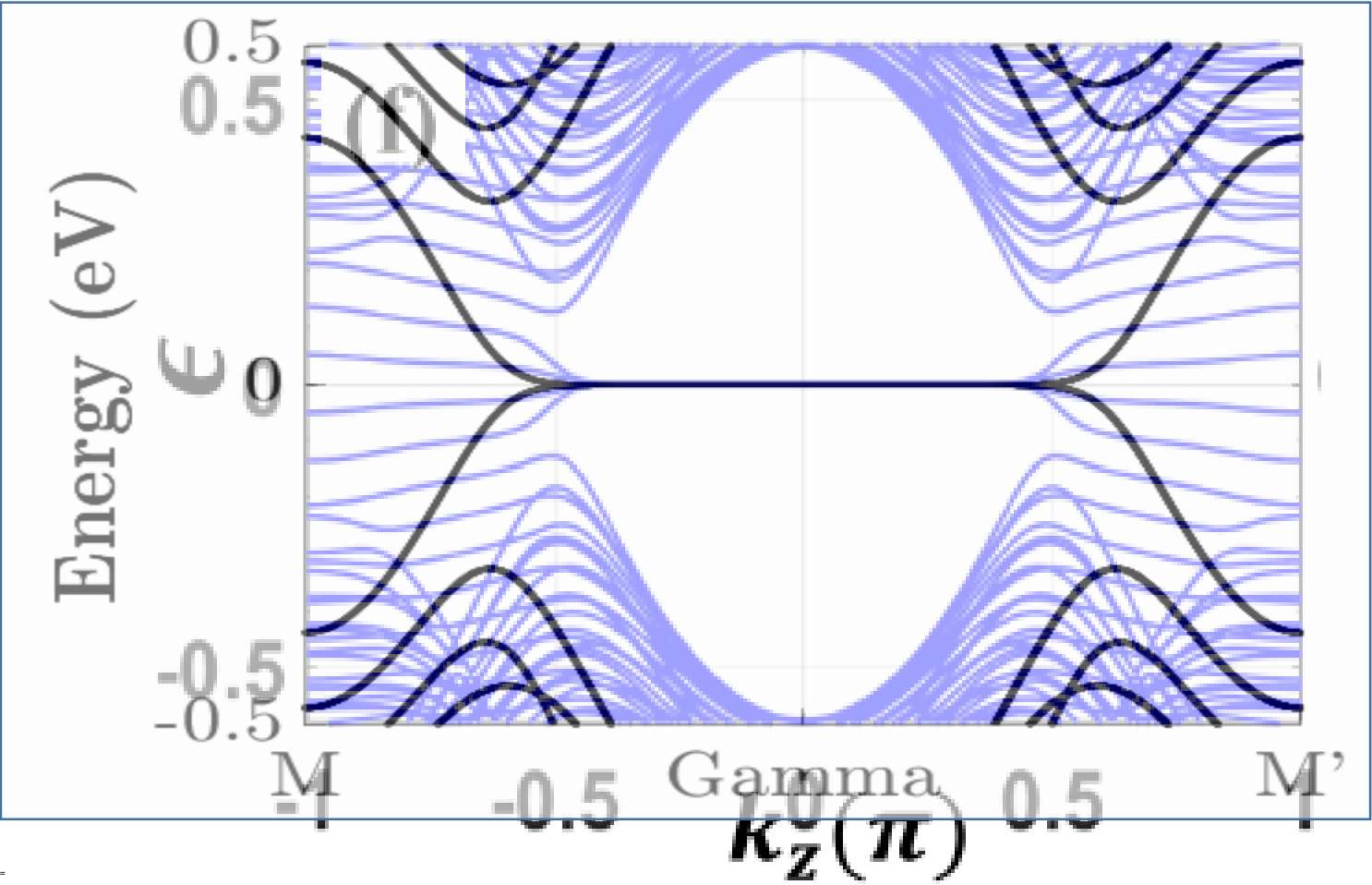
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gamma = -0.7;  
m1     = 0.6/sqrt(2);
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projection to k_z

bulk projection (3D \Rightarrow 1D)

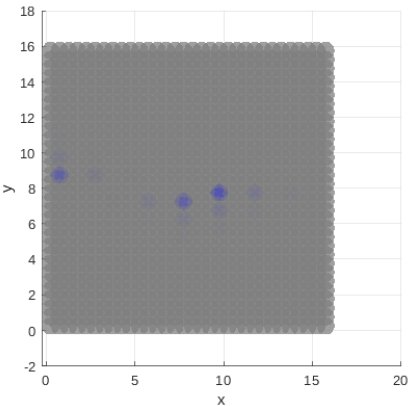
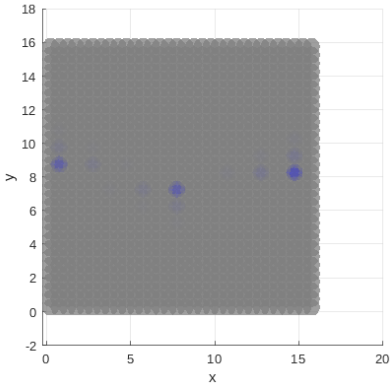


$$16L \times 16L$$

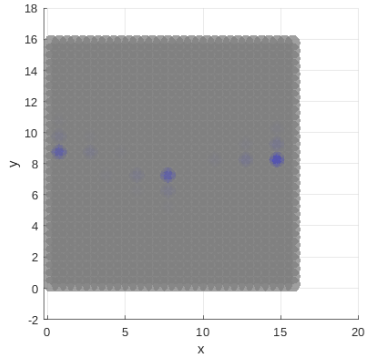


at $k_z = 0$

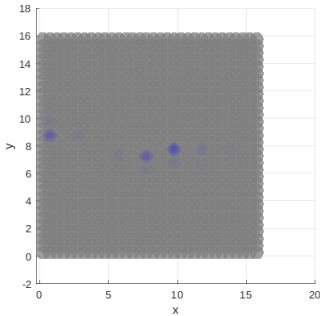
energy =
-8.8979e-12



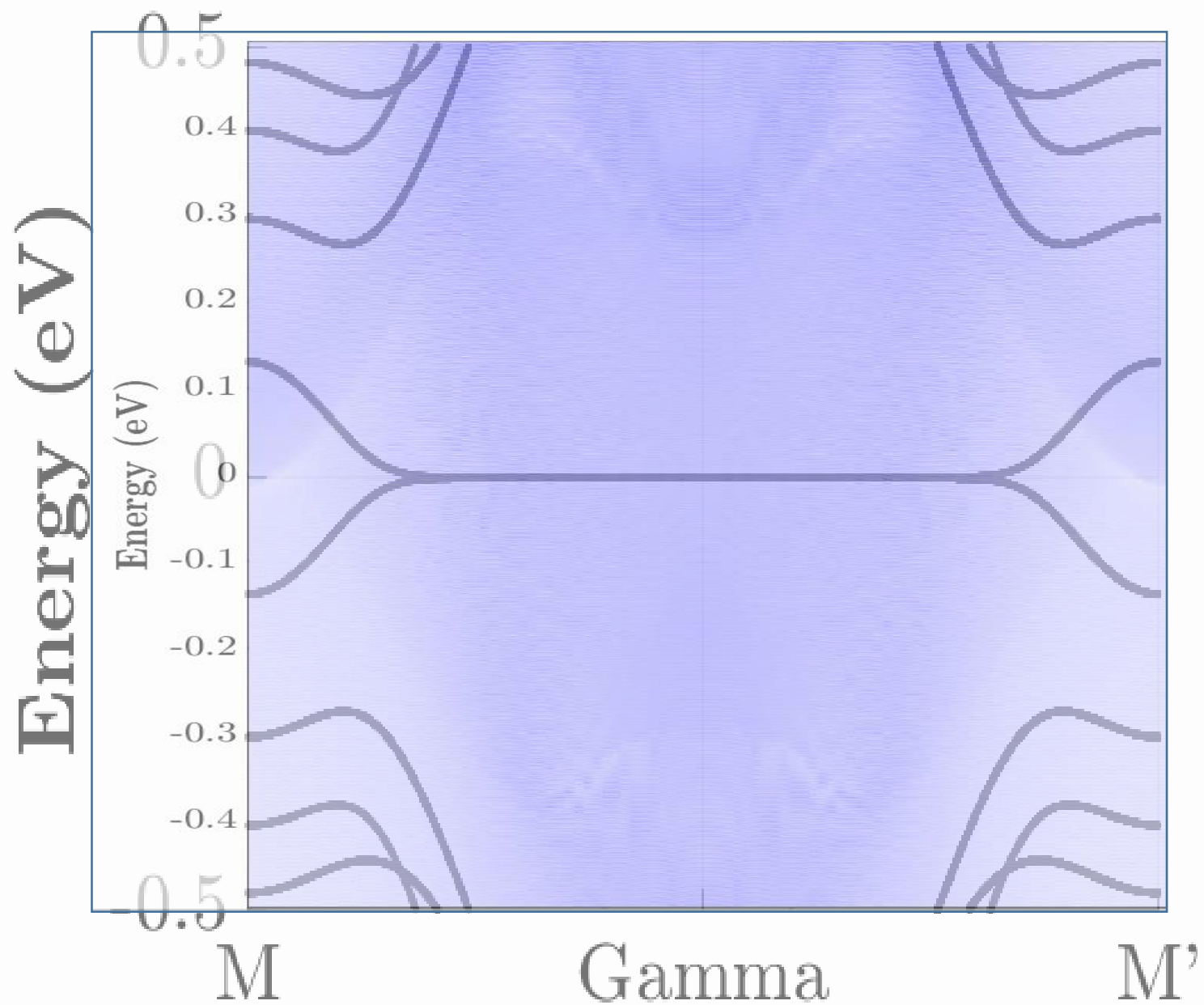
energy =
8.8970e-12



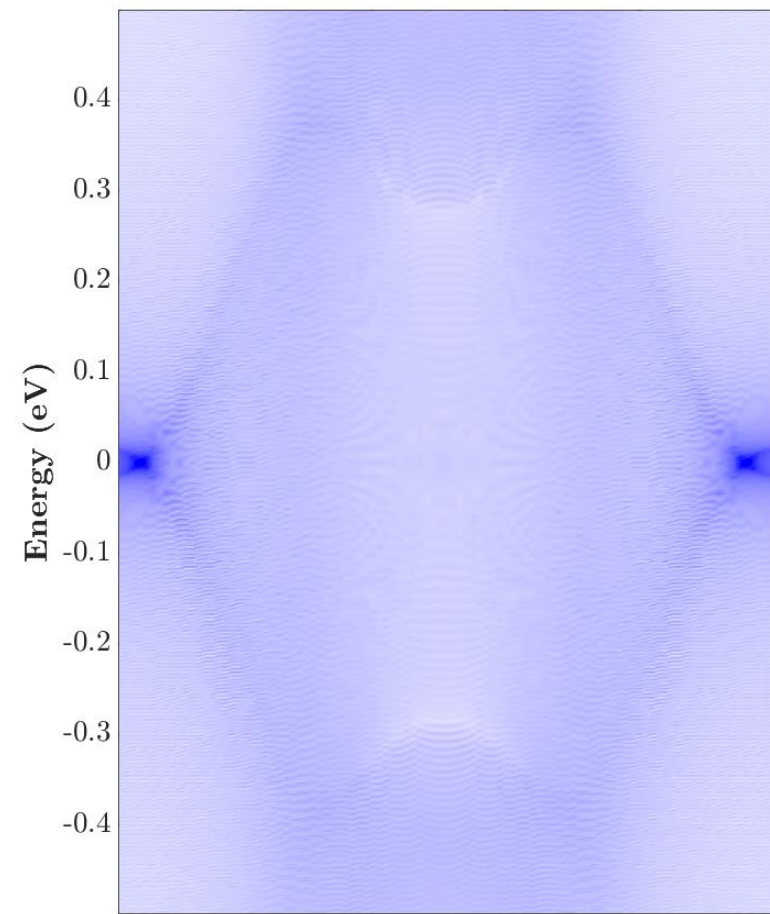
energy =
8.8973e-12



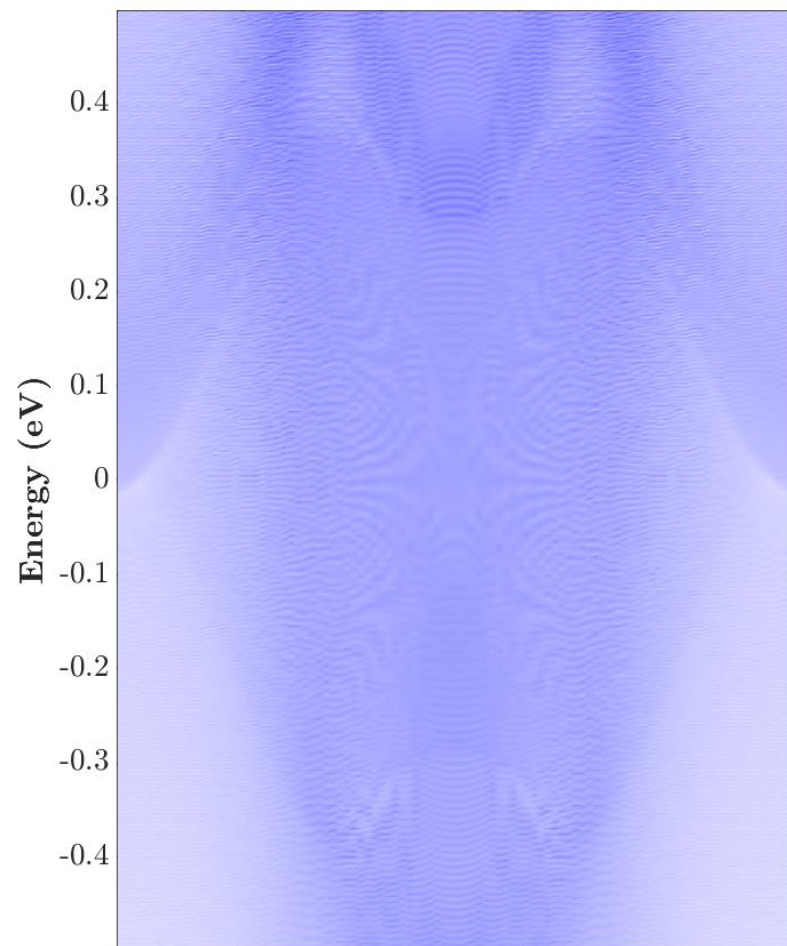
corner



eastS



southS



bulk

