Revisiting Quadratic Band Crossing: From Interaction-driven Instability to Intrinsic Topology

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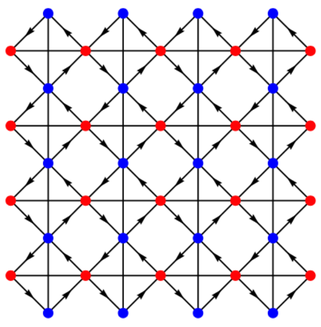
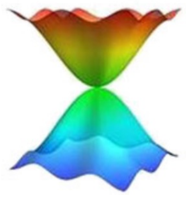
Introduction: QBCP to QAH

$$H = \int d\boldsymbol{r}\left[\Psi^\dagger(\boldsymbol{r})\mathcal{H}_0\Psi(\boldsymbol{r}) + V\psi_1^\dagger(\boldsymbol{r})\psi_1(\boldsymbol{r})\psi_2^\dagger(\boldsymbol{r})\psi_2(\boldsymbol{r})\right]$$

$$\Rightarrow [\text{mean field}]\int d\boldsymbol{r}\Psi^\dagger(\boldsymbol{r})\left[\mathcal{H}_0 - \frac{V}{2}\left(Q_S\sigma_z + Q_B\sigma_x + \phi_{QAH}\sigma_y\right)\right]\Psi(\boldsymbol{r}) + \frac{V}{4}\int d\boldsymbol{r}\left(Q_S^2 + Q_B^2 + \phi_{QAH}^2\right)$$

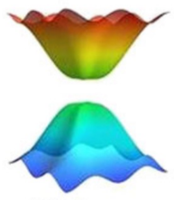


C_{4v}



QBCP

Interaction-driven symmetry breaking



QAH

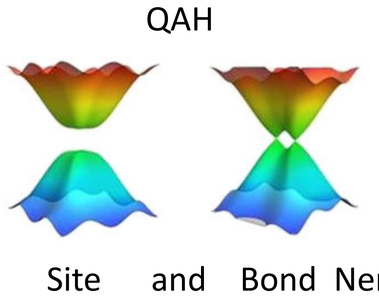
Order Parameters

$$\phi_{QAH} = \langle\Psi^\dagger(\boldsymbol{r})\sigma_y\Psi(\boldsymbol{r})\rangle$$

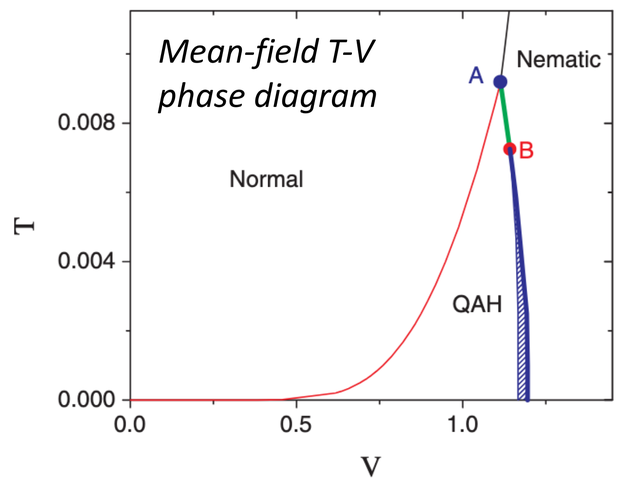
VS

$$Q_S = \langle\Psi^\dagger(\boldsymbol{r})\sigma_z\Psi(\boldsymbol{r})\rangle$$

$$Q_B = \langle\Psi^\dagger(\boldsymbol{r})\sigma_x\Psi(\boldsymbol{r})\rangle$$



Site and Bond Nematic



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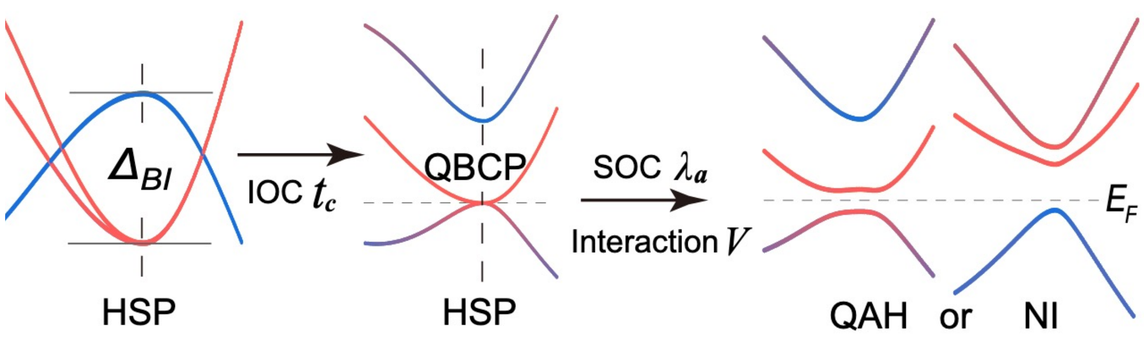
Three-orbitals Model and Electron Interactions

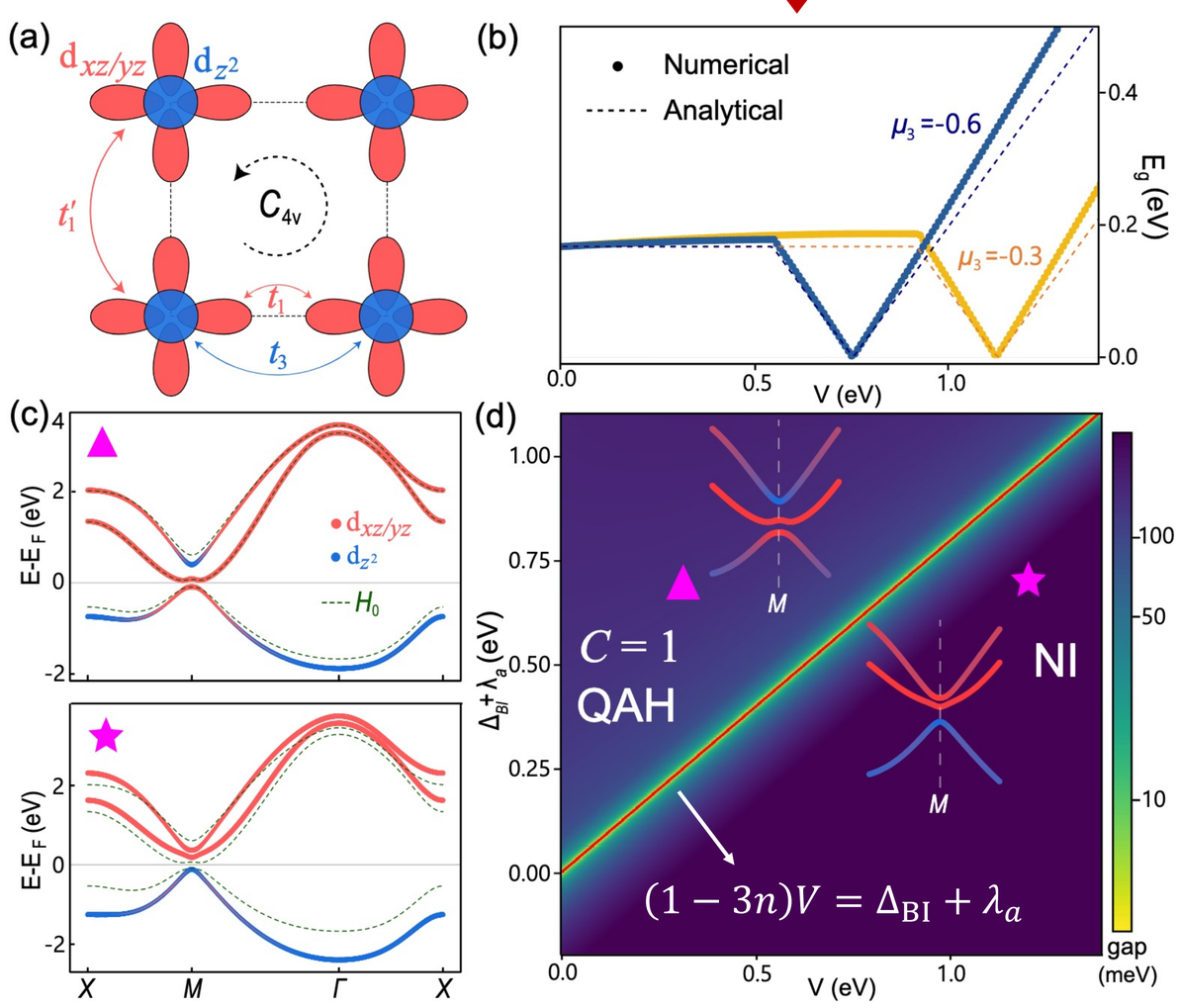


$$\mathcal{H}_0(k) = h_0 + h(\boldsymbol{k}) = \begin{pmatrix}\mu_1 & i\lambda_a & 0\\ -i\lambda_a & \mu_1 & 0\\ 0 & 0 & \mu_3\end{pmatrix} + \begin{pmatrix}h_1 & 0 & h_c\\ 0 & h_1' & h_c'\\ h_c^* & h_c^{*\prime} & h_3\end{pmatrix}$$

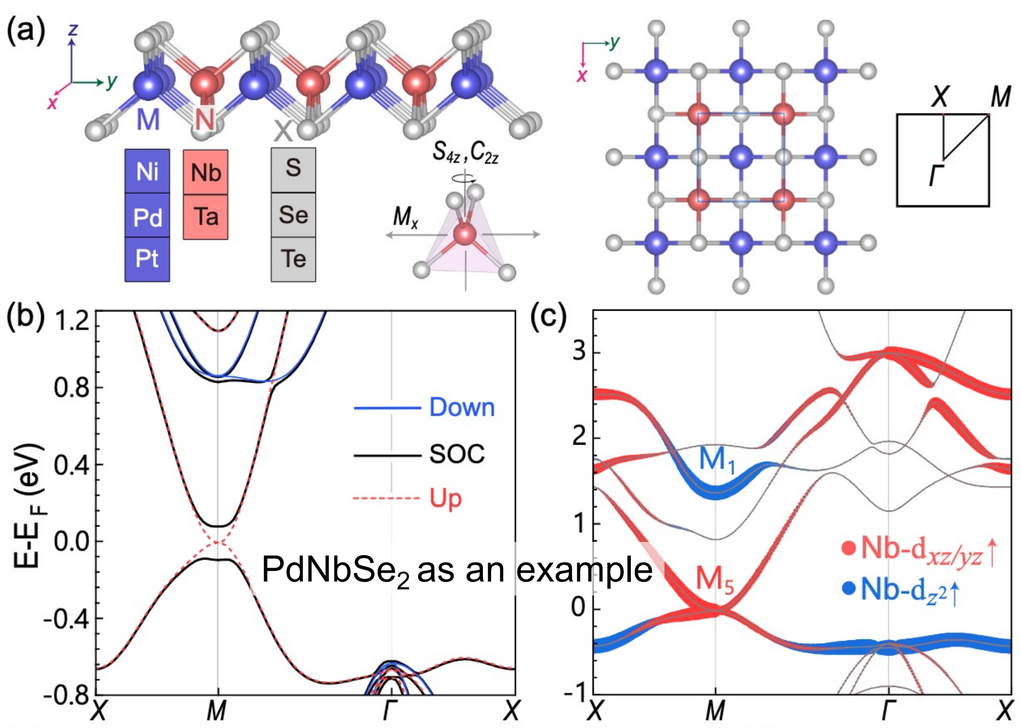
	$h^{\text{Tetr}}(\mathbf{k})$	$h^{\text{Tri}}(\mathbf{k})$
h_1	$t_1\cos k_x + t_1'\cos k_y$	$t_1\sum_{j=1}^{3}\cos(\mathbf{k}\cdot\boldsymbol{\delta}_j)$
h_1'	$t_1\cos k_y + t_1'\cos k_x$	
h_3	$t_3(\cos k_x + \cos k_y)$	$t_3\sum_{j=1}^{3}\cos(\mathbf{k}\cdot\boldsymbol{\delta}_j)$
h_c	$it_c\sin k_x$	$it_c\left[\sin(\mathbf{k}\cdot\boldsymbol{\delta}_1) - \frac{1}{2}\sum_{j=2}^{3}\sin(\mathbf{k}\cdot\boldsymbol{\delta}_j)\right]$
h_c'	$-it_c\sin k_y$	$-i\frac{\sqrt{3}}{2}t_c\left[\sin(\mathbf{k}\cdot\boldsymbol{\delta}_2) - \sin(\mathbf{k}\cdot\boldsymbol{\delta}_3)\right]$

$$\mathcal{H}_{int} = \sum_i V_1 n_{i,1}n_{i,2} + V_2\left(n_{i,1} + n_{i,2}\right)n_{i,3}$$

Hartree-Fock calculations



Candidate materials



	M_1	M_5
E	1	2
$2S_{4z}$	1	0
C_{2z}	1	-2
$2C_2'$	1	0
$2M_x$	1	0

Extension to C_{6v}