Artificial Lattice

Jan 24, 2019

Today’s discussion

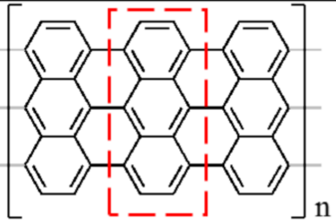
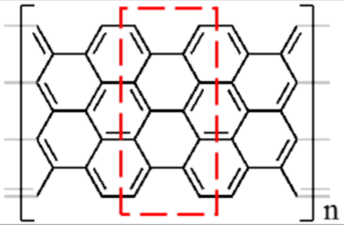
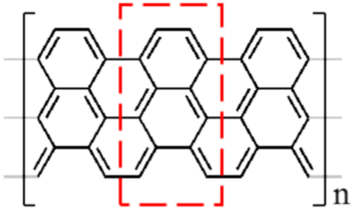
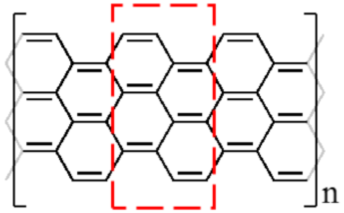
- Steven Louie paper on graphene nanoribbons
  - Analytical expression for Z2
  - Junction states at the interface between GNRs of two different width
  - Changing topological class by doping

Possible ways to compute “proxy” for topological invariant

  - Calculation of Zak phase using finite difference
  - Calculation of Z2 using Hybrid Wannier Charge Centers (implemented in Z2pack)

Topological phases in graphene nanoribbon (GNR)

- GNR with different width, edge and end termination belong to different electronic topological classes
- Topological phases of GNR is characterized by Z2 invariant (Z2 = 0 or 1)
- Explicit formula for Z2 invariant derived analytically by solving Tight Binding Hamiltonian for graphene

Termination type	Zigzag (N = Odd)	Zigzag' (N = Odd)	Zigzag (N = Even)	Bearded (N = Even)
Unit cell shape				
Bulk Symmetry	Inversion/mirror	Inversion/mirror	Mirror	Inversion
Z_2	$\frac{1+(-1)^{\lfloor \frac{N}{3} \rfloor + \lfloor \frac{N+1}{2} \rfloor}}{2}$	$\frac{1-(-1)^{\lfloor \frac{N}{3} \rfloor + \lfloor \frac{N+1}{2} \rfloor}}{2}$		$\frac{1-(-1)^{\lfloor \frac{N}{3} \rfloor}}{2}$

Tiang Cao, PRL, 2017

$$H^g(\boldsymbol{k}) = -t\begin{pmatrix} 0 & 1 + e^{ia\left(-\frac{\sqrt{3}}{2}k_x+\frac{1}{2}k_y\right)} + e^{ia\left(-\frac{\sqrt{3}}{2}k_x-\frac{1}{2}k_y\right)} \\ 1 + e^{ia\left(\frac{\sqrt{3}}{2}k_x+\frac{1}{2}k_y\right)} + e^{ia\left(\frac{\sqrt{3}}{2}k_x-\frac{1}{2}k_y\right)} & 0 \end{pmatrix},$$

Solving for the eigenvalues and eigenvectors

$$h_x(\boldsymbol{k}) = 1 + 2\cos\left(\frac{ak_y}{2}\right)\cos\left(\frac{\sqrt{3}ak_x}{2}\right),$$

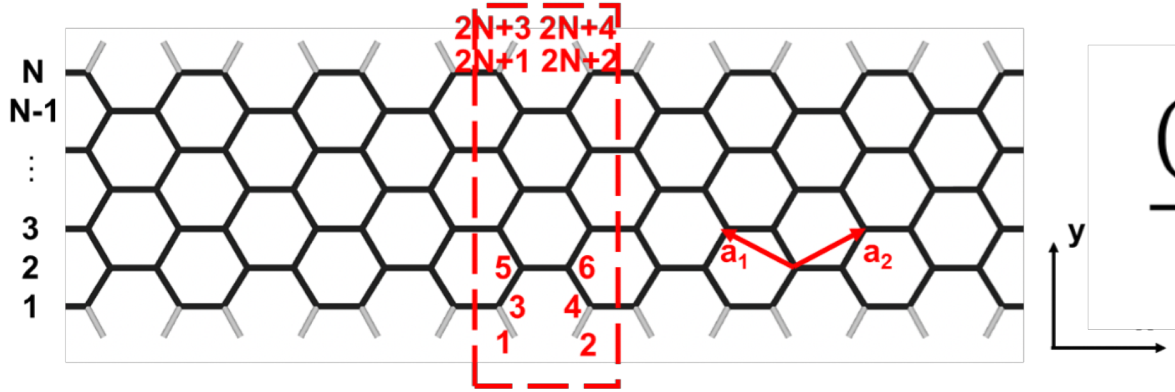
$$h_y(\boldsymbol{k}) = 2\cos\left(\frac{ak_y}{2}\right)\sin\left(\frac{\sqrt{3}ak_x}{2}\right).$$

$$E_\pm(\boldsymbol{k}) = \pm t\sqrt{h_x^2(\boldsymbol{k}) + h_y^2(\boldsymbol{k})},$$

$$u_\pm^g(\boldsymbol{k}) = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\phi(\boldsymbol{k})} \\ \mp 1 \end{pmatrix},$$

$$e^{-i\phi(\boldsymbol{k})} = \frac{h_x(\boldsymbol{k}) - ih_y(\boldsymbol{k})}{\sqrt{h_x^2(\boldsymbol{k}) + h_y^2(\boldsymbol{k})}}.$$

GNR



$$\frac{(N+1)a}{2} k_y(n) = n\pi,$$

Construct the WF of GNR as linear combination of (k_x, k_y) and $(k_x, -k_y)$ states

$$u_n(k_x) = \frac{1}{\sqrt{2}}\left[u^{\underline{g}}\left(k_x, k_y(n)\right) - u^{\underline{g}}\left(k_x, -k_y(n)\right)\right].$$

$$u_n\left(k_x, k_y(n)\right) = \frac{1}{\sqrt{N}} \begin{pmatrix} e^{-ik_x\frac{\sqrt{3}}{2}a} i \sin\left(k_y \frac{a}{2}\right) \\ e^{-i\phi(\boldsymbol{k})} e^{ik_x\frac{\sqrt{3}}{2}a} i \sin\left(k_y \frac{a}{2}\right) \\ e^{-i\phi(\boldsymbol{k})} i \sin(k_y a) \\ i \sin(k_y a) \\ \cdots \end{pmatrix}.$$

Wavefunctions at BZ center are eigenfunctions of parity operators

$$P u_n(\Gamma) = f_n(\Gamma) u_n(\Gamma).$$

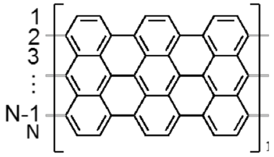
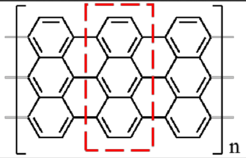
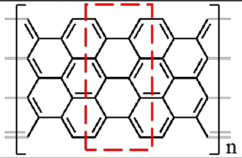
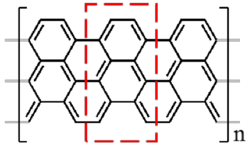
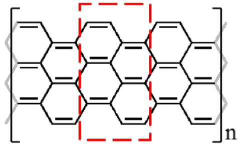
At X point $u_n(X)$ and $u_{N+1-n}(X)$ are orthogonal to each other. They form states with opposite parity.

$$p_n(\mathrm{X}) p_{N+1-n}(\mathrm{X}) = -1.$$

Topological insulators with inversion symmetry

Liang Fu, PRB (2007)

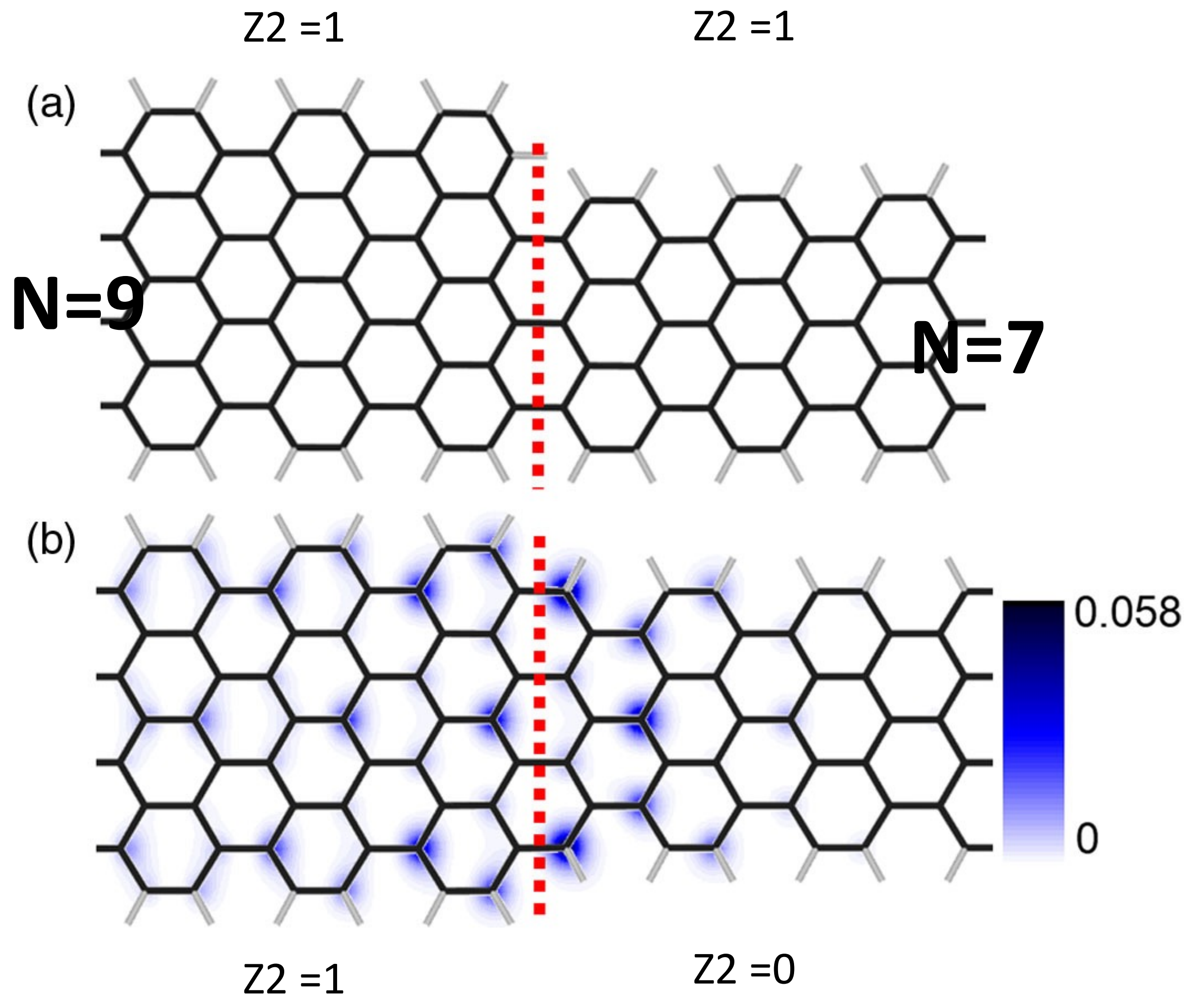
$$(-1)^{Z2} = \Pi_n p_n(\Gamma) p_n(X)$$

	N = Odd				N = Even			
Termination type	Zigzag		Zigzag'		Zigzag		Bearded	
Unit cell shape								
Bulk Symmetry	Inversion/mirror		Inversion/mirror		Mirror		Inversion	
N mod 12	1, 3, 11	5, 7, 9	1, 3, 11	5, 7, 9	0, 8, 10	2, 4, 6	4, 10	0, 2, 6, 8
Z_2	0	1	1	0	0	1	1	0

- Even and odd number of localized end states for Z=0 and Z2=1 respectively
- Confirmed by explicit DFT calculations in Ting Cao, 2017, PRL

Zigzag N=even does not have inversion symmetry!

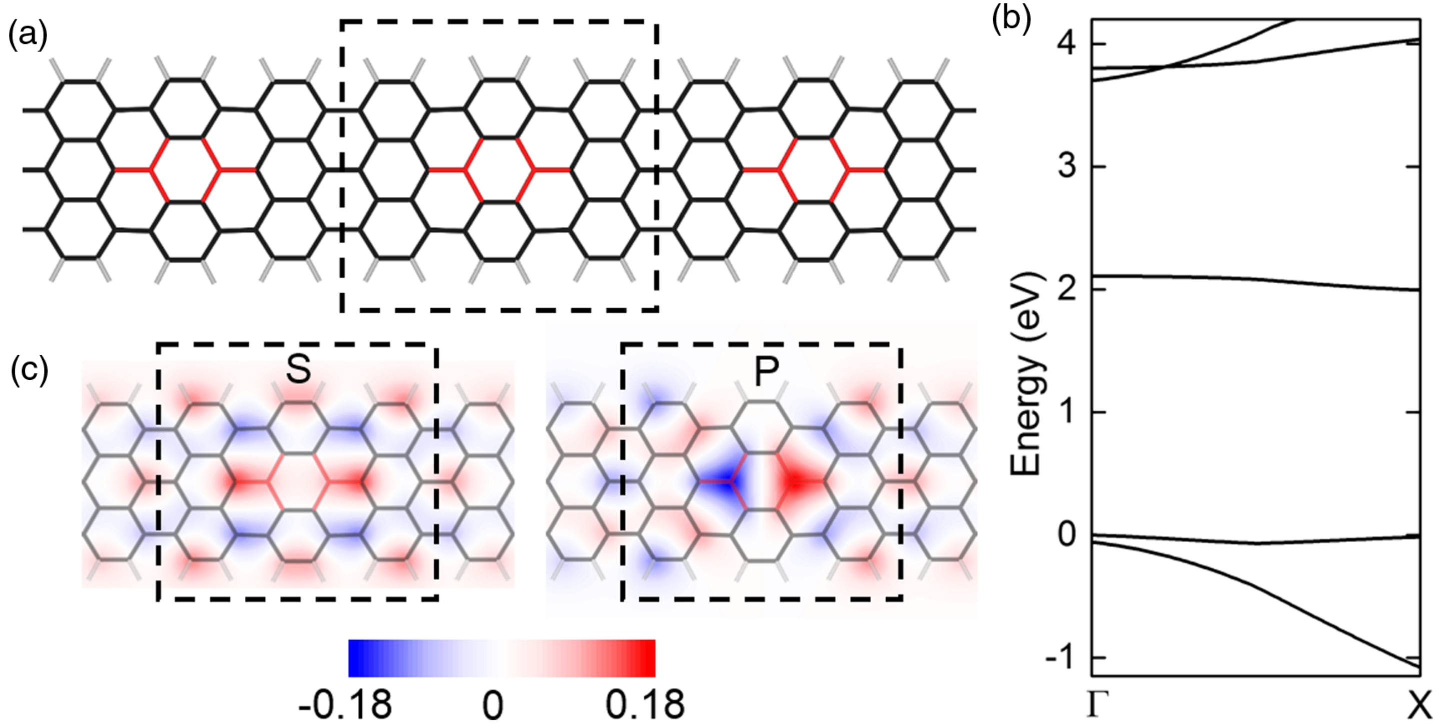
Junction States in GNR

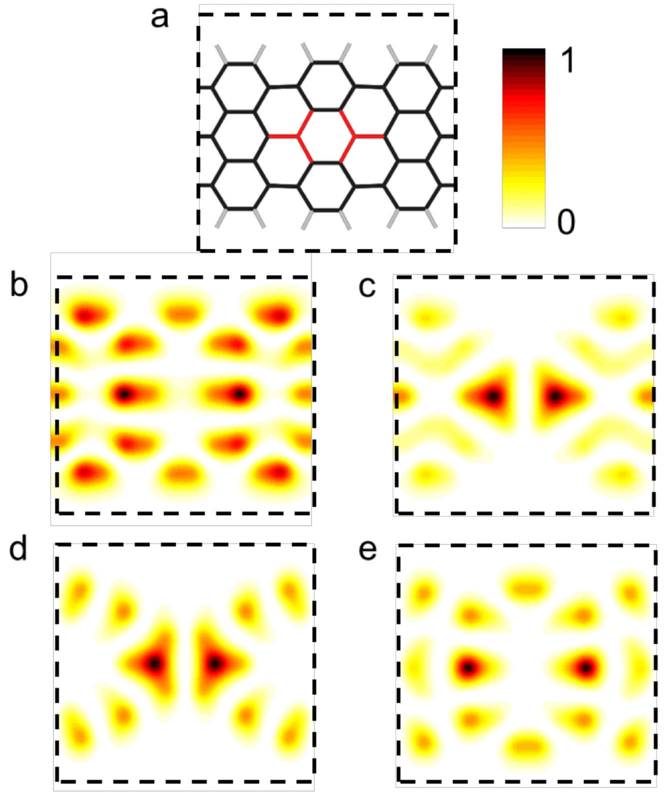


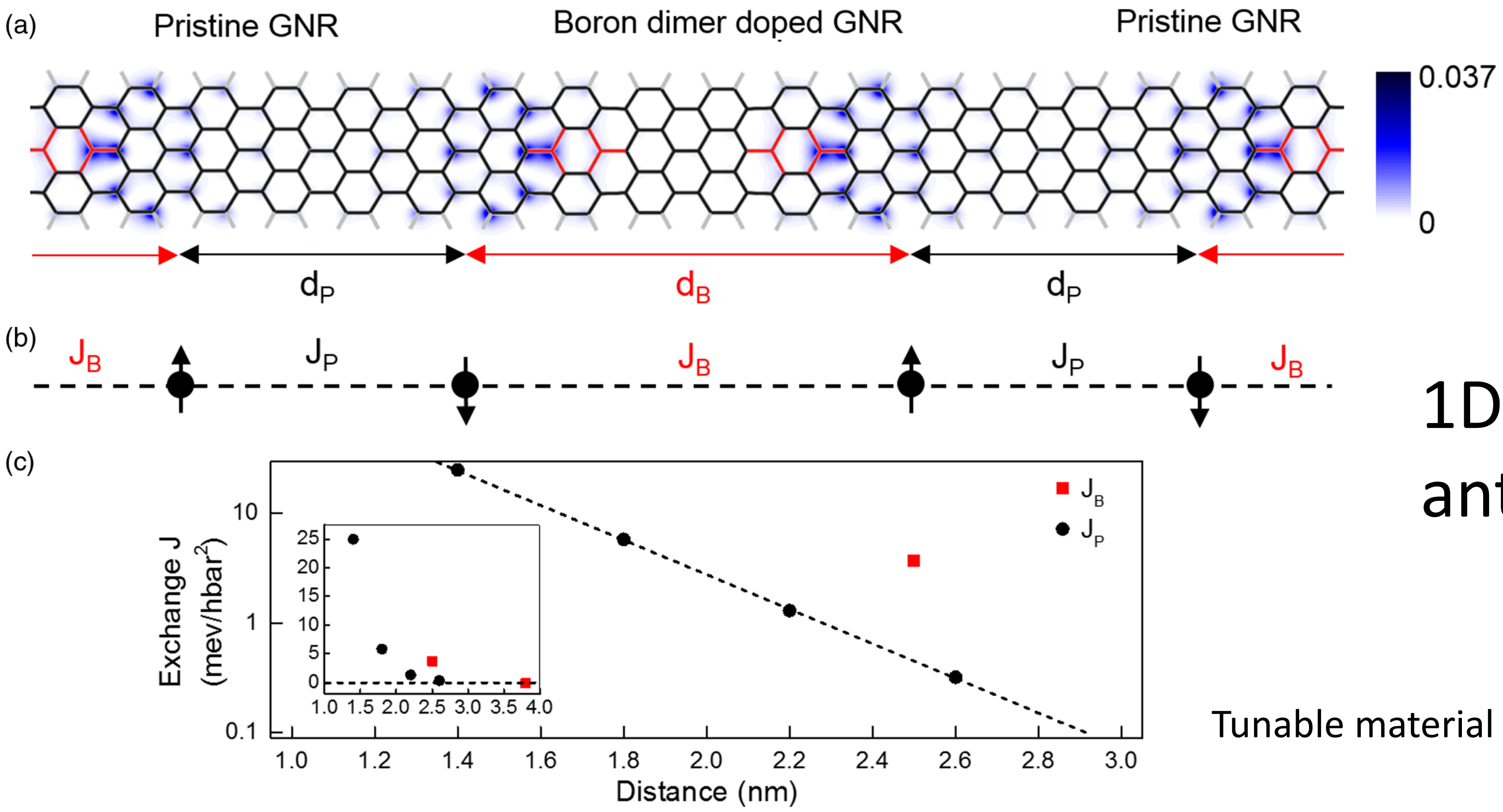
Termination of the N=7 GNR changes just by shifting the NR laterally
Z2 becomes 0

Bulk-edge correspondence

Changing topological class by doping







Midgap junction state acts as localized spin centers

1D Heisenberg antiferromagnetic chain

Tunable material platform

$$H = \Sigma_i [J_B(d_B) S_i^1 \cdot S_i^2 + J_P(d_P) S_i^2 \cdot S_{i+1}^1].$$

Finite difference to compute Zak phase

$$\gamma_n = i\left(\frac{2\pi}{d}\right)\int_{-\pi/d}^{\pi/d} dk \left\langle u_{nk}\left|\frac{\partial u_{nk}}{\partial k}\right.\right\rangle,$$

We only consider the 1D case

$P_n^{(\lambda)} = \frac{e}{2\pi}\Phi_n^{(\lambda)}$; L length of sample

$$\Phi_n^{(\lambda)} = -\mathrm{Im}\int_{\mathrm{BZ}} \mathrm{dk}\langle \mathrm{u}_{\mathrm{n,k}}^{(\lambda)}|\partial_{\mathrm{k}}|\mathrm{u}_{\mathrm{n,k}}^{(\lambda)}\rangle$$

Typically, we need to calculate this on a discrete grid of k-points

$$\int dk \langle u_{n,k}|\partial_k u_{n,k}\rangle dk \to \sum_{k_j} dk \langle u_{n,k}|\partial_k u_{n,k}\rangle|_{k=k_j}$$

Note the following:

$$u_{n,k+dk} \approx u_{n,k} + \partial_k u_{n,k}\, dk$$

$$\langle u_{n,k}|u_{n,k+dk}\rangle \approx 1 + \langle u_{n,k}|\partial_k u_{n,k}\rangle dk$$

Wilson loop

$$\ln[\langle u_{n,k}|u_{n,k+dk}\rangle] = \ln[1 + \langle u_{n,k}|\partial_k u_{n,k}\rangle dk] \approx \langle u_{n,k}|\partial_k u_{n,k}\rangle dk$$

Z2pack

Still experimenting with these methods.

PHYSICAL REVIEW B **95**, 075146 (2017)

Z2Pack: Numerical implementation of hybrid Wannier centers for identifying topological materials

Dominik Gresch,[1] Gabriel Autès,[2,3] Oleg V. Yazyev,[2,3] Matthias Troyer,[1] David Vanderbilt,[4]
B. Andrei Bernevig,[5] and Alexey A. Soluyanov[1,6]

[1] *Theoretical Physics and Station Q Zurich, ETH Zurich, 8093 Zurich, Switzerland*
[2] *Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland*
[3] *National Centre for Computational Design and Discovery of Novel Materials MARVEL, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland*
[4] *Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA*
[5] *Department of Physics, Princeton University, Princeton, New Jersey 08544, USA*
[6] *Department of Physics, St. Petersburg State University, St. Petersburg, 199034 Russia*

(Received 28 October 2016; revised manuscript received 13 December 2016; published 23 February 2017)

The intense theoretical and experimental interest in topological insulators and semimetals has established band structure topology as a fundamental material property. Consequently, identifying band topologies has become an important, but often challenging, problem, with no exhaustive solution at the present time. In this work we compile a series of techniques, some previously known, that allow for a solution to this problem for a large set of the possible band topologies. The method is based on tracking hybrid Wannier charge centers computed for relevant Bloch states, and it works at all levels of materials modeling: continuous $\mathbf{k} \cdot \mathbf{p}$ models, tight-binding models, and *ab initio* calculations. We apply the method to compute and identify Chern, $\mathbb{Z}_2$, and crystalline topological insulators, as well as topological semimetal phases, using real material examples. Moreover, we provide a numerical implementation of this technique (the Z2Pack software package) that is ideally suited for high-throughput screening of materials databases for compounds with nontrivial topologies. We expect that our work will allow researchers to (a) identify topological materials optimal for experimental probes, (b) classify existing compounds, and (c) reveal materials that host novel, not yet described, topological states.