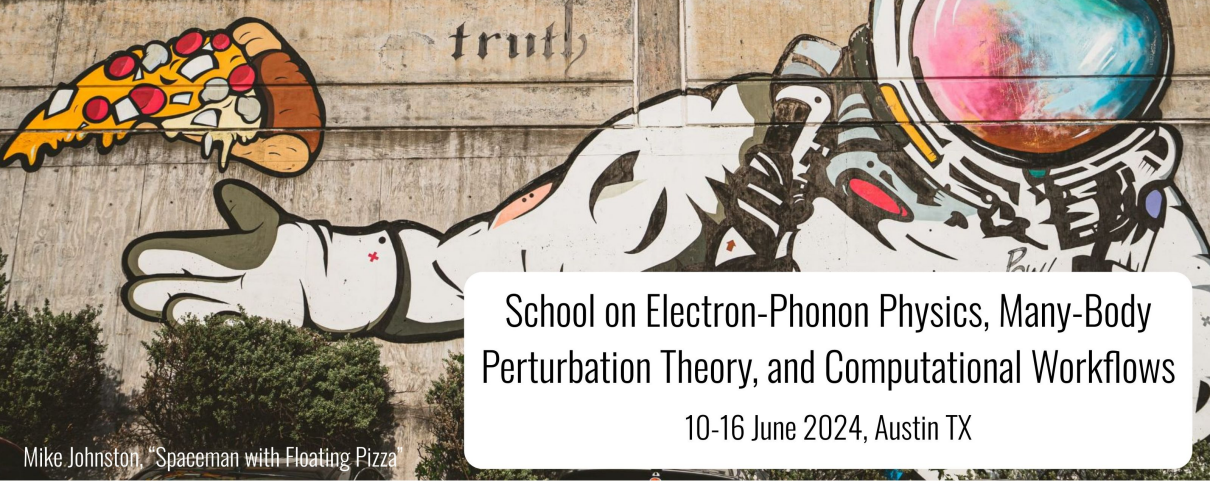


Mike Johnston, "Spaceman with Floating Pizza"

School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows

10-16 June 2024, Austin TX

U.S. DEPARTMENT OF ENERGY

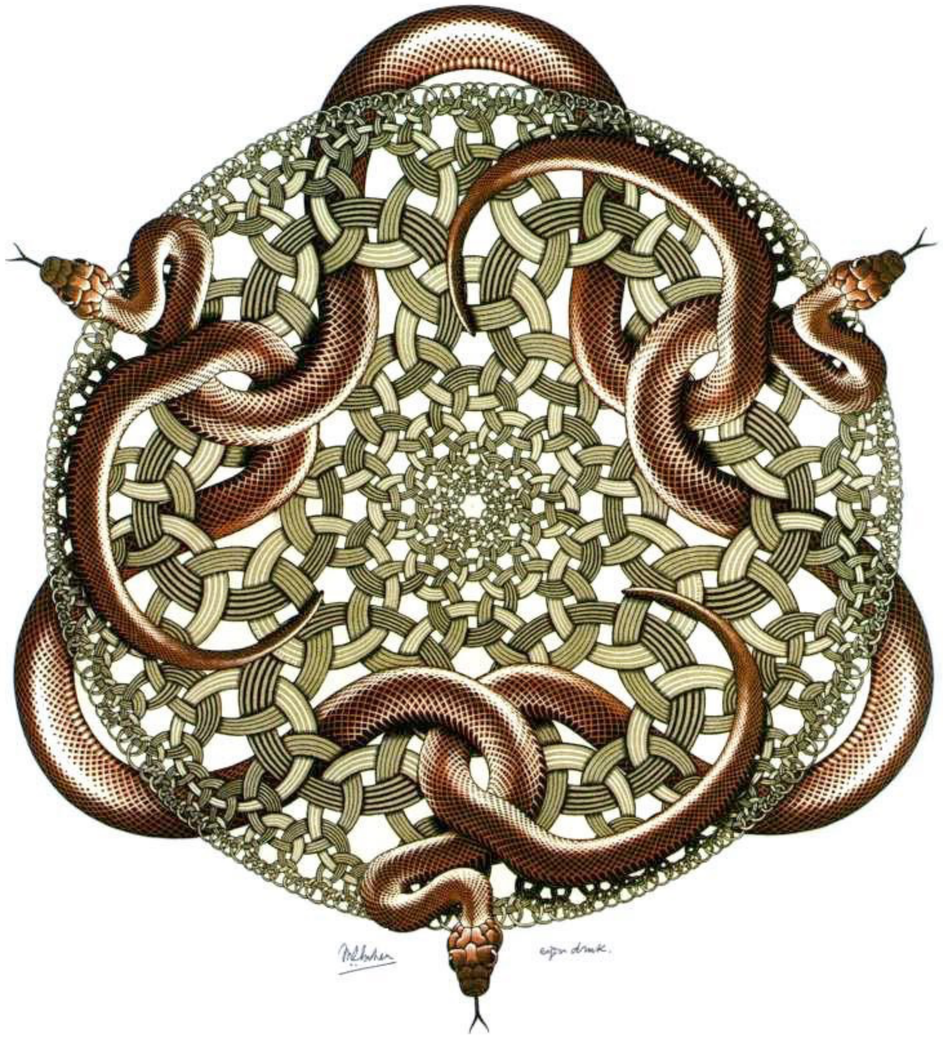
NSF

TACC
TEXAS ADVANCED COMPUTING CENTER

ODEN

Making mountains out of molehills, and other tails of disentanglement

Nicola Marzari, EPFL and PSI



Electronic structure – a personal history

J. Phys. C: Solid State Phys., Vol. 12, 1979. Printed in Great Britain. © 1979

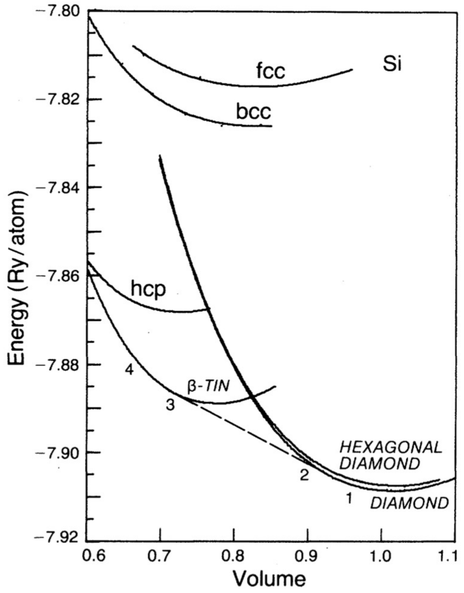
Momentum-space formalism for the total energy of solids

J Ihm, Alex Zunger and Marvin L Cohen†

Department of Physics, University of California and Materials and Molecular Research Division, Lawrence Berkeley Laboratory, Berkeley, California 94720, USA

Received 8 May 1979

$$E_{\text{total}} = \Omega\Bigg(\sum_{i,\boldsymbol{G}} |\psi(\boldsymbol{k}_i + \boldsymbol{G})|^2 (\boldsymbol{k}_i + \boldsymbol{G})^2 + \tfrac{1}{2}\sum_{\boldsymbol{G}} V_{\text{Coul}}(\boldsymbol{G})\,\rho(\boldsymbol{G}) + \tfrac{3}{4}\sum_{\boldsymbol{G}} \mu_{\text{xc}}(\boldsymbol{G})\,\rho(\boldsymbol{G}) + \sum_{\boldsymbol{G}} S(\boldsymbol{G})\,U_{\text{ps}}(\boldsymbol{G})\,\rho(\boldsymbol{G}) + \sum_{i,l,\boldsymbol{G},\boldsymbol{G}'} \psi^*(\boldsymbol{k}_i + \boldsymbol{G})\,\psi(\boldsymbol{k}_i + \boldsymbol{G}')\,S(\boldsymbol{G}' - \boldsymbol{G}) \times U'_{\text{ps},\,l,\,\boldsymbol{k}_i+\boldsymbol{G},\,\boldsymbol{k}_i+\boldsymbol{G}'}\Bigg) + \tfrac{1}{2}\sum_{\substack{\mu,\nu \\ \mu\neq\nu}} \frac{2Z^2}{|\boldsymbol{R}_\mu - \boldsymbol{R}_\nu|}.$$



VOLUME 45, NUMBER 12 PHYSICAL REVIEW LETTERS 22 SEPTEMBER 1980

Microscopic Theory of the Phase Transformation and Lattice Dynamics of Si

M. T. Yin and Marvin L. Cohen

Department of Physics, University of California, Berkeley, California 94720, and Materials and Molecular Research Division, Lawrence Berkeley Laboratory, Berkeley, California 94720

(Received 14 July 1980)

An *ab initio* calculation for the solid-solid phase transformation, static structural properties, and the lattice dynamics of Si is presented. A density-functional pseudopotential scheme is used with the atomic number as the only input. The detailed properties of the diamond to β-tin transition are accurately reproduced. The phonon frequencies and mode-Grüneisen parameters at Γ and X, along with the lattice constant, bulk modulus, and cohesive energy, are calculated and found to be in excellent agreement with experiment.

Electronic structure – a personal history

PHYSICAL REVIEW B VOLUME 26, NUMBER 8 15 OCTOBER 1982

Pseudopotentials that work: From H to Pu

G. B. Bachelet,* D. R. Hamann, and M. Schlüter
Bell Laboratories, Murray Hill, New Jersey 07974
(Received 28 April 1982)

VOLUME 55, NUMBER 22 PHYSICAL REVIEW LETTERS 25 NOVEMBER 1985

Unified Approach for Molecular Dynamics and Density-Functional Theory

R. Car
International School for Advanced Studies, Trieste, Italy
and
M. Parrinello
Dipartimento di Fisica Teorica, Università di Trieste, Trieste, Italy, and International School for Advanced Studies, Trieste, Italy
(Received 5 August 1985)

We present a unified scheme that, by combining molecular dynamics and density-functional theory, profoundly extends the range of both concepts. Our approach extends molecular dynamics beyond the usual pair-potential approximation, thereby making possible the simulation of both covalently bonded and metallic systems. In addition it permits the application of density-functional theory to much larger systems than previously feasible. The new technique is demonstrated by the calculation of some static and dynamic properties of crystalline silicon within a self-consistent pseudopotential framework.

PACS numbers: 71.10.+x, 65.50.+m, 71.45.Gm

VOLUME 58, NUMBER 18 PHYSICAL REVIEW LETTERS 4 MAY 1987

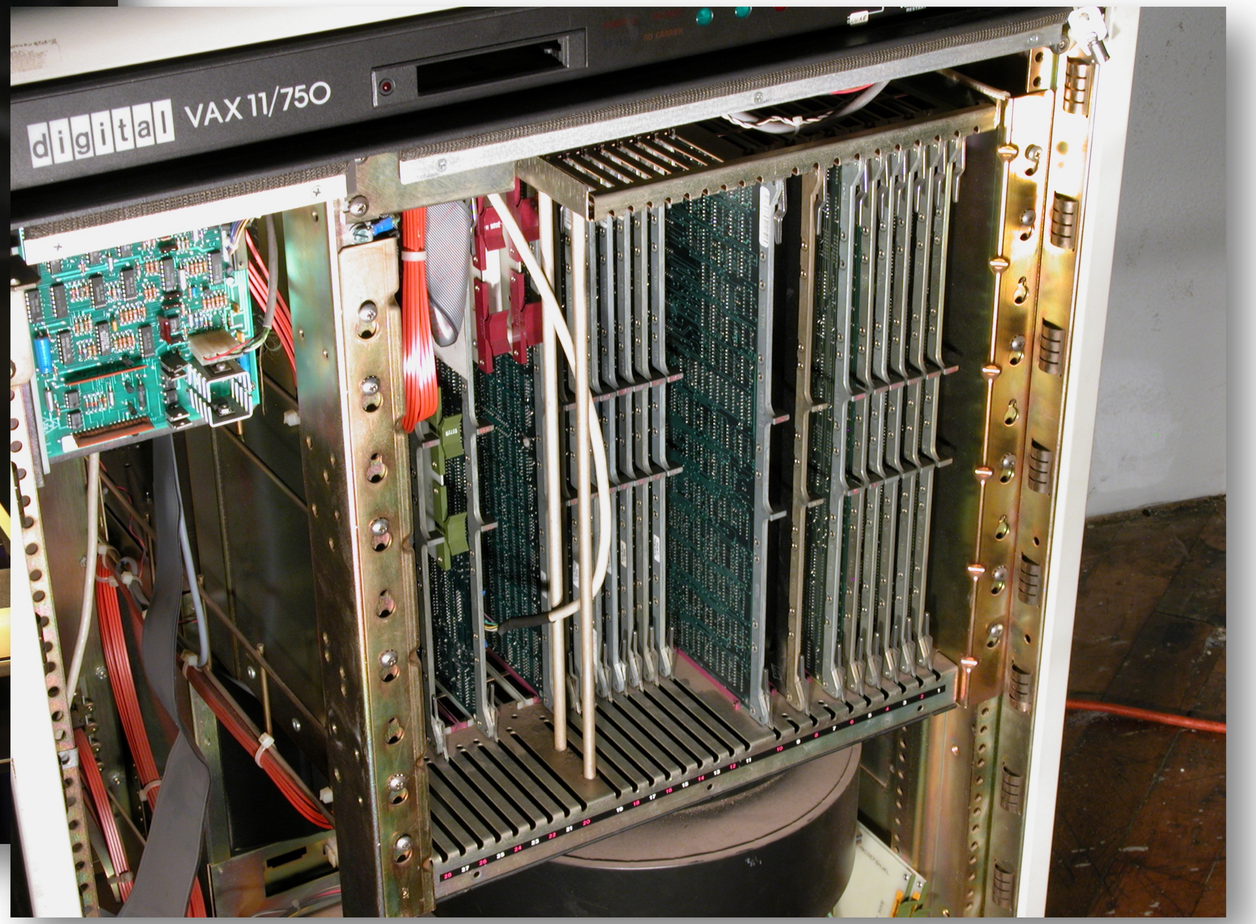
Green's-Function Approach to Linear Response in Solids

Stefano Baroni
Dipartimento di Fisica Teorica, Università di Trieste, I-34014 Trieste, Italy
Paolo Giannozzi
Institut de Physique Théorique, Université de Lausanne, BSP-Dorigny, CH-1015 Lausanne, Switzerland
and
Andrea Testa
Institut de Physique Théorique, Ecole Polytechnique Fédérale de Lausanne, PHB-Ecublens, CH-1015 Lausanne, Switzerland
(Received 24 February 1987)

We present a new scheme to study the linear response of crystals which combines the advantages of the dielectric-matrix and supercell ("direct") approaches yet avoids many of their drawbacks. The numerical complexity of the algorithm is of the same order as that of a self-consistent calculation for the *unperturbed* system. The method is not restricted to local perturbations as is the dielectric-matrix one nor to short wavelength as is the direct one. As an application, we calculate the long-wavelength optical phonons in Si and GaAs, both transverse and longitudinal, using norm-conserving pseudopotentials, and without any use of supercells.

PACS numbers: 63.10.+a, 71.10.+x, 77.90.+k

Digital VT100, VAX 11/750



The sky is the limit

EUROPHYSICS LETTERS

Europhys. Lett., 17 (6), pp. 547-552 (1992)

1 February bis 1992

published in January 1992

Towards Very Large-Scale Electronic-Structure Calculations.

S. BARONI (*) and P. GIANNOZZI (**)

(*) *Scuola Internazionale Superiore di Studi Avanzati (SISSA)*
Via Beirut 4, I-34014 Trieste, Italy
(**) *Scuola Normale Superiore - Piazza dei Cavalieri 7, I-56100 Pisa, Italy*

VOLUME 69, NUMBER 24 PHYSICAL REVIEW LETTERS 14 DECEMBER 1992

Large Scale Electronic Structure Calculations

Giulia Galli[(1),(2)] and Michele Parrinello[(2)]
[(1)] *Institut Romand de Recherche Numérique en Physique des Matériaux (IRRMA), PHB Ecublens, 1015 Lausanne, Switzerland*[(a)]
[(2)] *IBM Research Division, Zurich Research Laboratory, 8803 Rüschlikon, Switzerland*
(Received 26 May 1992)

1993 Seattle APS March Meeting

PHYSICAL REVIEW B VOLUME 47, NUMBER 16 15 APRIL 1993-II

Density-matrix electronic-structure method with linear system-size scaling

X.-P. Li, R. W. Nunes, and David Vanderbilt
Department of Physics and Astronomy, Rutgers University, P.O. Box 849, Piscataway, New Jersey 08855-0849
(Received 27 July 1992)

RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 47, NUMBER 15 15 APRIL 1993-I

Rapid Communications

Rapid Communications are intended for the accelerated publication of important new results and are therefore given priority treatment both in the editorial office and in production. A Rapid Communication in **Physical Review B** *should be no longer than four printed pages and must be accompanied by an abstract. Page proofs are sent to authors.*

Orbital formulation for electronic-structure calculations with linear system-size scaling

Francesco Mauri, Giulia Galli, and Roberto Car
Institut Romand de Recherche Numérique en Physique des Matériaux (IRRMA), PHB-Ecublens, 1015 Lausanne, Switzerland
(Received 19 January 1993)

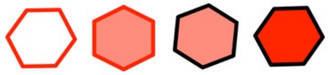
PHYSICAL REVIEW B VOLUME 48, NUMBER 19 15 NOVEMBER 1993-I

Unconstrained minimization approach for electronic computations that scales linearly with system size

Pablo Ordejón
Department of Physics, University of Illinois, Urbana, Illinois 61801

David A. Drabold
Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701-2979

Matthew P. Grumbach and Richard M. Martin
Department of Physics, University of Illinois, Urbana, Illinois 61801
(Received 8 March 1993)



Pelléas et Melisande, and the UK speed limit

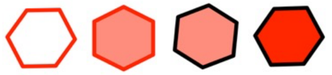
Home > Performance Database > Pelléas et Mélisande > Pelléas et Mélisande (1993) > Search Results

Pelléas et Melisande-29 March 1993 Evening 7.30pm

First| Previous| 3 of 6 performances| Next| Last| List All

Opera: Performance details

Company:	The Royal Opera
Venue:	Royal Opera House, Covent Garden, London
Performance status:	Original season
Conductor	Claudio Abbado
Chorus Director	Terry Edwards
Leader	John Brown



Rutgers, and linear scaling

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CISE Postdoctoral Research Associates in Computational Science
and Engineering
and
CISE Postdoctoral Research Associates in Experimental Computer
Science

Program Announcement

DIVISION OF ADVANCED SCIENTIFIC COMPUTING
AND
OFFICE OF CROSS-DISCIPLINARY ACTIVITIES

DEADLINE: NOVEMBER 1, 1995

NATIONAL SCIENCE FOUNDATION

CISE Postdoctoral Research Associates in Computational
Science and Engineering
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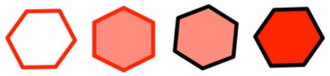

Rutgers, and linear scaling

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CISE Postdoctoral Research Associates in Experimental Computer Science

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NATIONAL SCIENCE FOUNDATION

CISE Postdoctoral Research Associates in Computational Science and Engineering

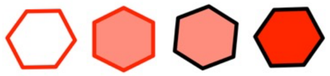
Date: Thu, 19 Oct 1995 15:55:13 -0400
From: David Vanderbilt <dhv@physics.rutgers.edu>
Message-Id: <199510191955.PAA04323@plasmon.rutgers.edu>
To: nm10007@cam.ac.uk
Subject: proposal
Status: OR

Nicola,

Thanks for sending the draft.

> I guess that your first impressions would be very useful...

I think it is basically very good;



Rutgers, and linear scaling

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CISE Postdoctoral Research Associates in Experimental Computer Science

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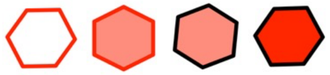

Rutgers, and linear scaling

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Subject: proposal
Status: OR

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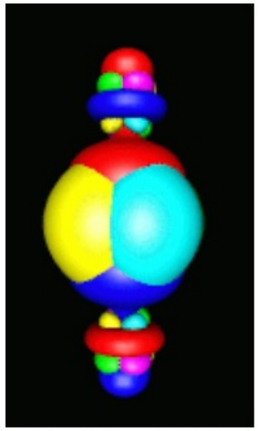
Postdoc: Research Training for CS&E Postdoctoral Associate in Electronic Structure Theory

NSF Org:	OAC Office of Advanced Cyberinfrastructure (OAC)
Awardee:	RUTGERS, THE STATE UNIVERSITY OF NEW JERSEY
Initial Amendment Date:	August 14, 1996

FOCUS

Nobel Focus: Chemistry by Computer

October 21, 1998 • *Phys. Rev. Focus* 2, 19



Nicola Marzari and David Vanderbilt/Rutgers University

Calculations made easy. Localized orbitals in the electronic structure of the $BaTiO_3$ crystal, calculated using density functional theory, which was invented by 1998 Nobel Laureate Walter Kohn.

Self-Consistent Equations Including Exchange and Correlation Effects
W. Kohn and L. J. Sham
Phys. Rev. 140, A1133 (1965)
Published November 15, 1965

Inhomogeneous Electron Gas
P. Hohenberg and W. Kohn
Phys. Rev. 136, B864 (1964)
Published November 9, 1964

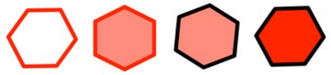
Recent Articles

Cecam 1999: Recent Developments in the Theory of Wannier Functions and Other Localized Electronic Wavefunctions

Bloch theorem

The one-particle effective Hamiltonian $\hat{H}$ in a periodic lattice commutes with the lattice-translation operator $\hat{T}_{\mathrm{R}}$, allowing us to choose the common eigenstates according to the prescriptions of Bloch theorem:

$$[\,\hat{H},\,\hat{T}_{\mathrm{R}}\,] \;=\; 0 \quad\Rightarrow\quad \Psi_{n\mathbf{k}}(\mathbf{r}) \;=\; u_{n\mathbf{k}}(\mathbf{r})\, e^{i\mathbf{k}\cdot\mathbf{r}}$$



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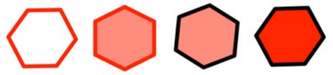
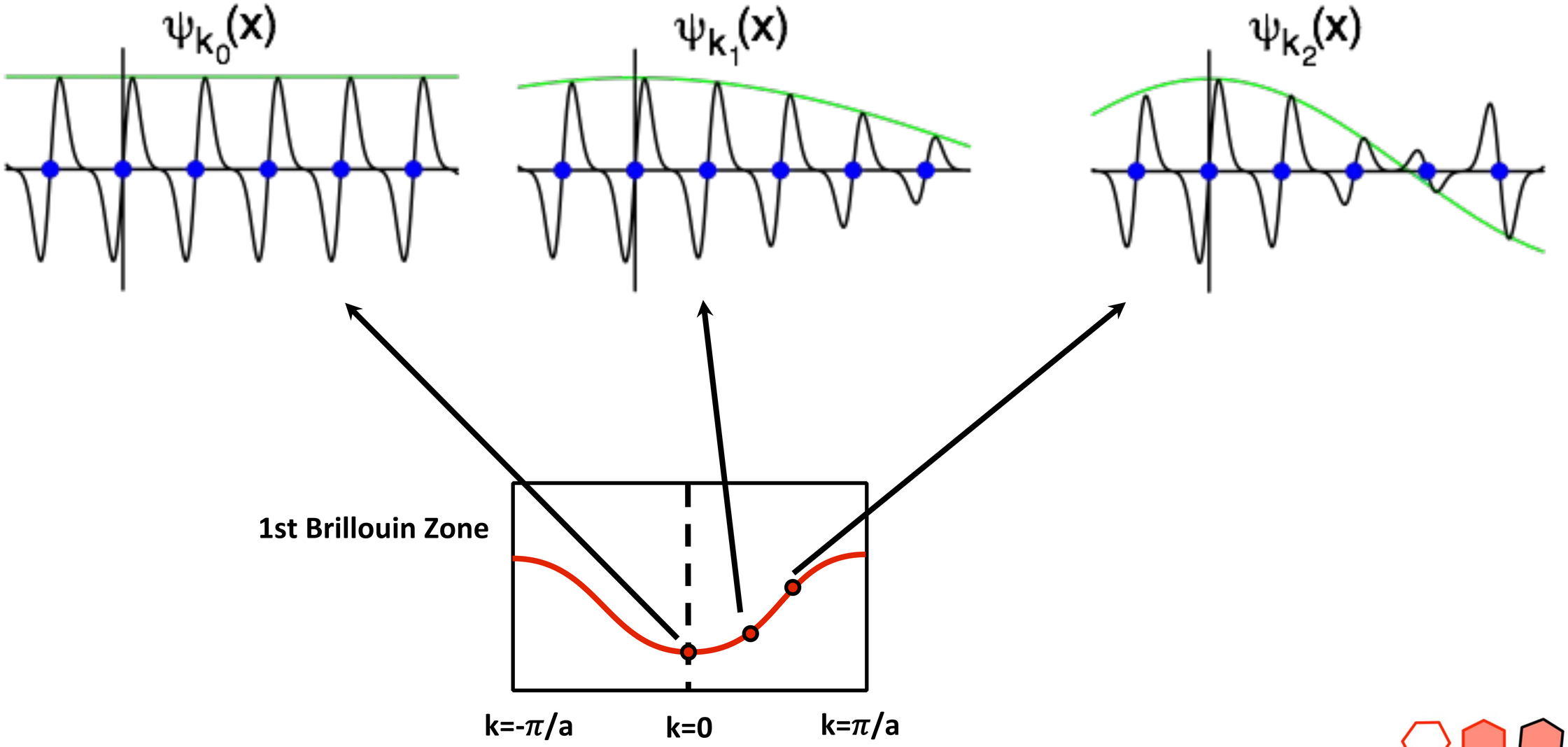
$$[\,\hat{H},\,\hat{T}_{\mathrm{R}}\,] \;=\; 0 \quad\Rightarrow\quad \Psi_{n\mathbf{k}}(\mathbf{r}) \;=\; u_{n\mathbf{k}}(\mathbf{r})\,e^{i\mathbf{k}\cdot\mathbf{r}}$$

- *n, k* are the quantum numbers (band index and crystal momentum), *u* is periodic
- From two requirements: a translation can't change the charge density, and two translations must be equivalent to one that is the sum of the two

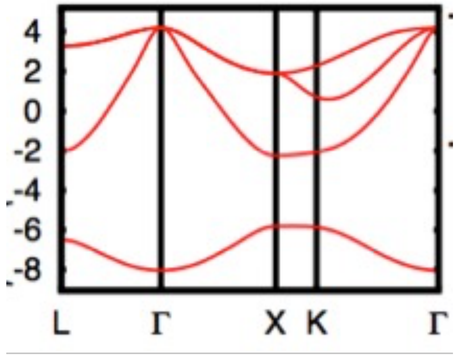


Bloch wavefunctions in 1d



From Bloch orbitals to Wannier functions

$$|\mathbf{R}n\rangle = \int_{BZ} \Psi_{n\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$



Gauge freedoms

- Arbitrary phase factor for every $n\mathbf{k}$ (Schrödinger)

$$|\mathbf{R}n\rangle = \int_{BZ} \left[e^{i\phi_n(\mathbf{k})}\psi_{n\mathbf{k}}(\mathbf{r})\right] e^{-i\mathbf{k}.\mathbf{R}} d\mathbf{k}$$

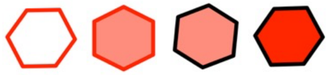
Long-range decay (heuristic…)

Isolated band, Wannier function around the origin

$$w_{\mathbf{0}}(\mathbf{r}) \;=\; \int_{BZ} \Psi_{\mathbf{k}}(\mathbf{r})\, d\mathbf{k} \;=\; \int_{BZ} u_{\mathbf{k}}(\mathbf{r})\, e^{i\mathbf{k}\cdot\mathbf{r}}\, d\mathbf{k}$$

For $\mathbf{r} \to \infty, \mathbf{r} = \mathbf{R}_i$

$$w_{\mathbf{0}}(\mathbf{R}_i) \;=\; \int_{BZ} u_{\mathbf{k}}(0)\, e^{i\mathbf{k}\cdot\mathbf{R}_\mathbf{i}}\, d\mathbf{k}$$

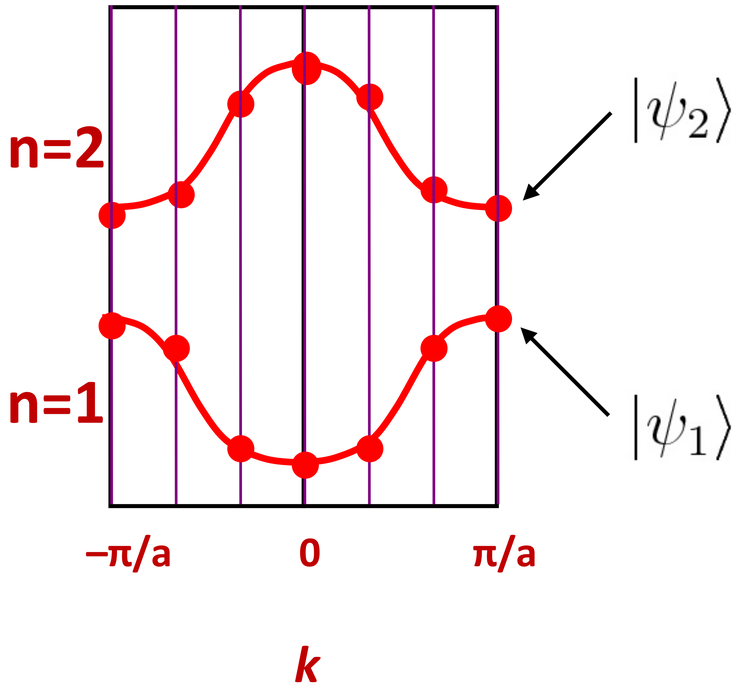


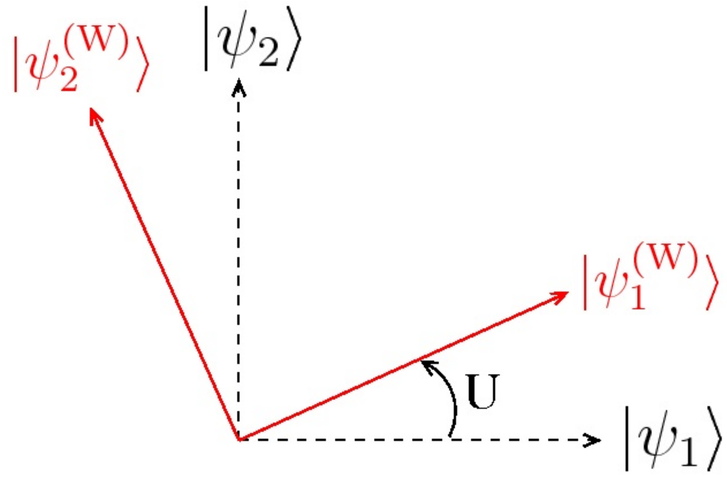
Unitary transformations

$$|\psi_{n\mathbf{k}}^{(\mathrm{W})}\rangle = \sum_m |\psi_{m\mathbf{k}}\rangle U_{mn}^{(\mathbf{k})}$$

Rotated Bloch function

Unitary matrix





From Bloch orbitals to Wannier functions

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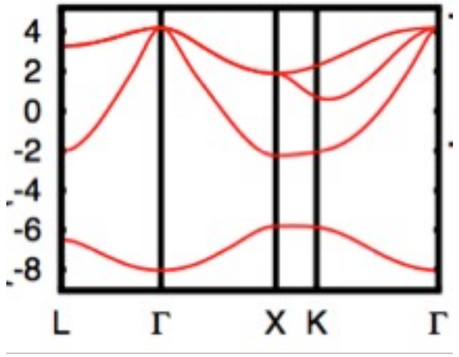


Gauge freedoms

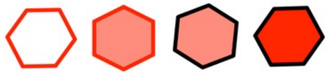
- Arbitrary phase factor for every $n\mathbf{k}$ (Schrödinger)
- Arbitrary unitary rotations $U^{(\mathbf{k})}_{mn}$ for every $\mathbf{k}$ (DFT)

$$|\mathbf{R}n\rangle = \int_{BZ} \sum_m U^{(\mathbf{k})}_{mn}\, \Psi_{m\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$

Generalized Wannier functions for composite bands

$$|\mathbf{R}n\rangle = \int_{BZ} \sum_{m} U^{(\mathbf{k})}_{mn} \Psi_{m\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$

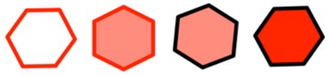
- $\{|\mathbf{R}n\rangle\}$ span the same space as $\{|\Psi_{n\mathbf{k}}\rangle\}$
- $|\mathbf{R}n\rangle = w_n(\mathbf{r}-\mathbf{R})$ (translational images)
- $\langle \mathbf{R}n|\mathbf{R}'m\rangle = \delta_{n,m}\,\delta_{\mathbf{R},\mathbf{R}'}$



Generalized Wannier functions for composite bands

$$|\mathbf{R}n\rangle = \int_{BZ} \sum_{m} U_{mn}^{(\mathbf{k})} \Psi_{m\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$

But how to choose U?



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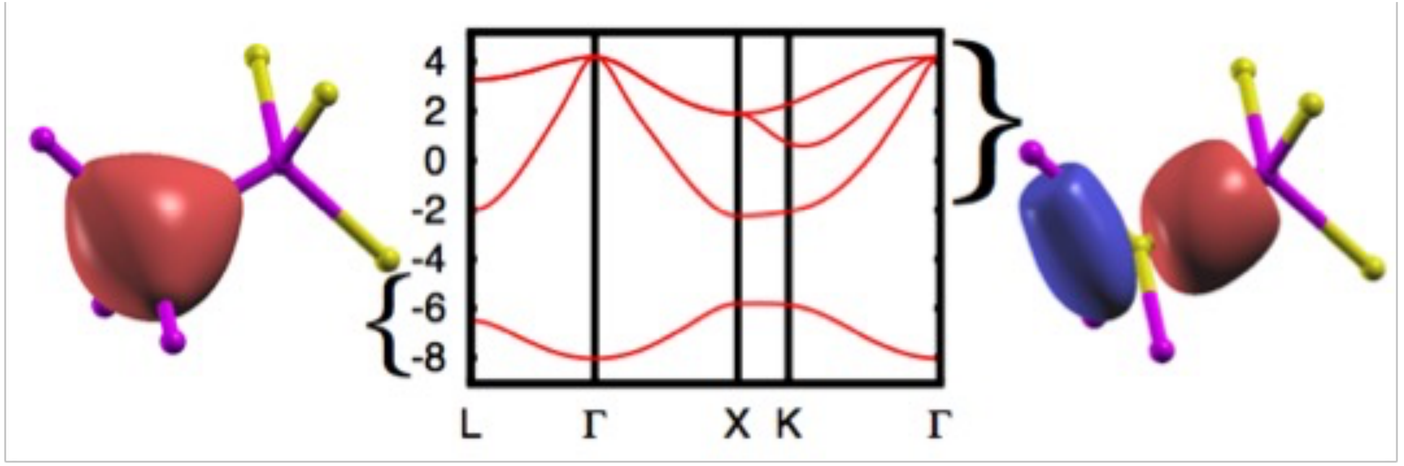
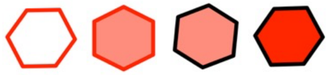


U and WFs by projection

A simple route is to obtain U through a projection onto a pre-defined set of local orbitals g_n

$$|\phi_{n\mathbf{k}}\rangle = \sum_{m=1}^{J} |\psi_{m\mathbf{k}}\rangle\langle\psi_{m\mathbf{k}}|g_n\rangle$$



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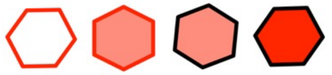
Can we choose U without reference to predetermined states?

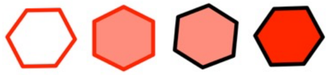


U and WFs by localization

$$\Omega = \sum_n \left[\langle \mathbf{0}n | r^2 | \mathbf{0}n \rangle - \langle \mathbf{0}n | \mathbf{r} | \mathbf{0}n \rangle^2 \right]$$

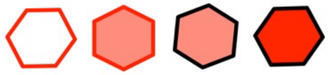
For a given set of Bloch orbitals, our goal is to minimize Ω with respect all the sets of unitary transformations $U_{mn}^{(\mathbf{k})}$

N. Marzari and D. Vanderbilt, Phys. Rev. B 56, 12847 (1997)



Outline

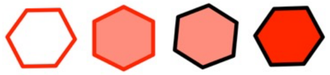
$$|\mathbf{R}n\rangle = \int_{BZ} \sum_{m} U_{mn}^{(\mathbf{k})} \Psi_{m\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$



Outline

$$|\mathbf{R}n\rangle = \int_{BZ} \sum_{m} U_{mn}^{(\mathbf{k})} \Psi_{m\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$

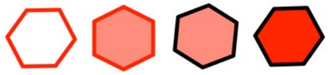
Bloch states from favourite electronic-structure code



Outline

$$|\mathbf{R}n\rangle = \int_{BZ} \sum_{m} U_{mn}^{(\mathbf{k})} \Psi_{m\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$

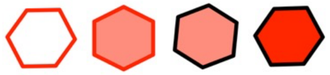
2 unitary transformations



Outline

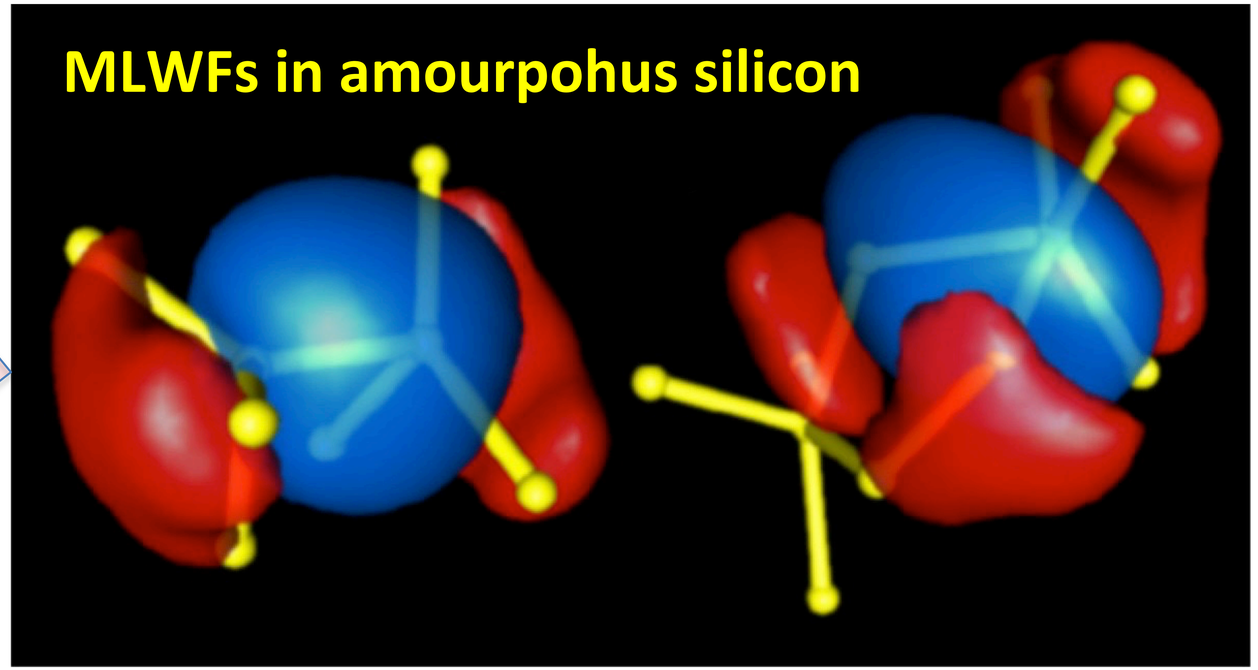
$$|\mathbf{R}n\rangle = \int_{BZ} \sum_{m} U_{mn}^{(\mathbf{k})} \Psi_{m\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$

Iteratively refine $U_{mn}^{(k)}$ to localize |Rn>



Outline

$$|\mathbf{R}n\rangle = \int_{BZ} \sum_{m} U_{mn}^{(\mathbf{k})} \, \Psi_{m\mathbf{k}}(\mathbf{r}) \, e^{-i\mathbf{k}\cdot\mathbf{R}} \, d\mathbf{k}$$



Decomposition of the localization functional

$$\Omega = \sum_n \left[\langle \mathbf{0}n | r^2 | \mathbf{0}n \rangle - \langle \mathbf{0}n | \mathbf{r} | \mathbf{0}n \rangle^2 \right]$$

$$\Omega_{\rm I} = \sum_n \left[\langle r^2 \rangle_n - \sum_{\mathbf{R}m} \left| \langle \mathbf{R}m | \mathbf{r} | \mathbf{0}n \rangle \right|^2 \right] \quad ,$$

$$\widetilde{\Omega} = \sum_n \sum_{\mathbf{R}m \neq \mathbf{0}n} \left| \langle \mathbf{R}m | \mathbf{r} | \mathbf{0}n \rangle \right|^2 \quad .$$

$\Omega_{\rm I}$ and $\widetilde{\Omega}$ are *positive-definite* and $\Omega_{\rm I}$ is *gauge-invariant !*

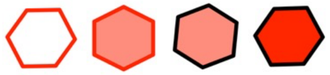
Ω_I is gauge invariant, positive definite

projection operators $\mathbb{P} = \sum_{\mathbf{R}m} |\mathbf{R}m\rangle\langle\mathbf{R}m|$ and $\mathbb{Q} = \mathbb{I} - \mathbb{P}$

$$\Omega_{\rm I} = \sum_n \left[\langle r^2 \rangle_n - \sum_{\mathbf{R}m} \left| \langle \mathbf{R}m|\mathbf{r}|0n\rangle \right|^2 \right] =$$

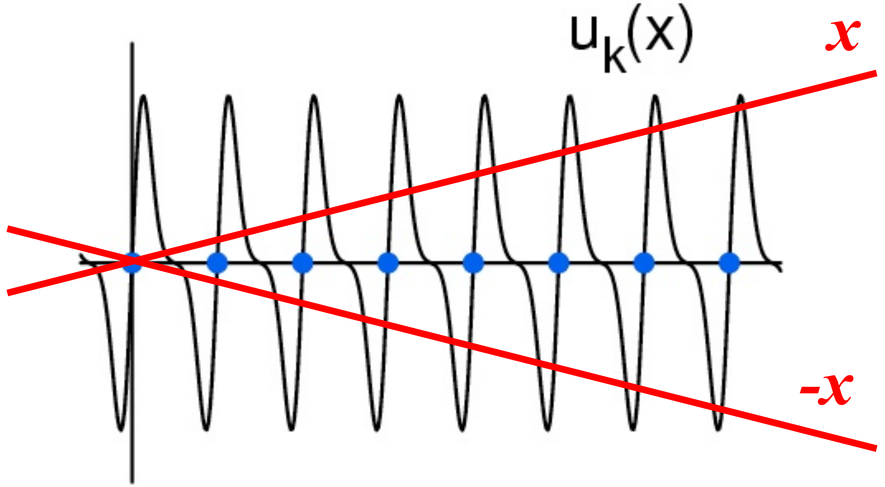
$$= \sum_{n,\alpha} \langle 0n|r_\alpha r_\alpha|0n\rangle_n - \sum_{n,\alpha} \left[\sum_{\mathbf{R}m} \langle 0n|r_\alpha|\mathbf{R}m\rangle\langle \mathbf{R}m|r_\alpha|0n\rangle \right] =$$

$$= \sum_{n,\alpha} \langle 0n|r_\alpha(\mathbb{I}-\mathbb{P})r_\alpha|0n\rangle = \sum_\alpha {\rm tr}_{\rm c}[r_\alpha \mathbb{Q}\, r_\alpha] = \sum_\alpha \|\mathbb{P} r_\alpha \mathbb{Q}\|_{\rm c}^2$$



Position operator is ill defined !

$$\langle \psi_k | x | \psi_k \rangle = \int_{-\infty}^{\infty} x \, |u_k(x)|^2 \, dx$$



But we know the position operator!

Original Articles

Theory of the electric polarization in crystals

R. Resta

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Download citation https://doi.org/10.1080/00150199208016065

RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 47, NUMBER 3 15 JANUARY 1993-I

Theory of polarization of crystalline solids

R. D. King-Smith and David Vanderbilt

Department of Physics and Astronomy, Rutgers University, P. O. Box 849, Piscataway, New Jersey 08855-0849

(Received 10 June 1992)

We consider the change in polarization $\Delta\mathbf{P}$ which occurs upon making an adiabatic change in the Kohn-Sham Hamiltonian of the solid. A simple expression for $\Delta\mathbf{P}$ is derived in terms of the valence-band wave functions of the initial and final Hamiltonians. We show that physically $\Delta\mathbf{P}$ can be interpreted as a displacement of the center of charge of the Wannier functions. The formulation is successfully applied to compute the piezoelectric tensor of GaAs in a first-principles pseudopotential calculation.

Blount identities

Centers of Wannier functions:

$$|\,w_0\rangle = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\;|\psi_{\mathbf{k}}\rangle$$

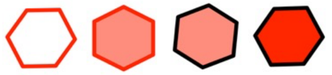
$$= \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\;e^{i\mathbf{k}\cdot\mathbf{r}}\,|u_{\mathbf{k}}\rangle$$

$$\mathbf{r}\,|\,w_0\rangle = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\;(\;-i\nabla_{\mathbf{k}}\,e^{i\mathbf{k}\cdot\mathbf{r}}\,)\,|u_{\mathbf{k}}\rangle$$

$$= i\,\frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\;e^{i\mathbf{k}\cdot\mathbf{r}}\,(\,\nabla_{\mathbf{k}}\,|u_{\mathbf{k}}\rangle\,)$$

$$\boxed{\langle w_0\,|\,\mathbf{r}\,|\,w_0\rangle = i\,\frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\;\langle u_{\mathbf{k}}|\,\nabla_{\mathbf{k}}\,|u_{\mathbf{k}}\rangle}$$

E. I. Blount, Solid State Physics 13, 305 (1962)



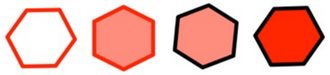
The reciprocal space representation

a) we need to be able to calculate derivatives on regular meshes in k-space; i f cubic symmetry is assumed, with each of the N k-points having $Z = 6, 8$ or 12 first-neighbors $\mathbf{k} + \mathbf{b}$, then:

$$\nabla f(\mathbf{k}) \;=\; \frac{3}{Zb^2} \sum_{\mathbf{b}} \mathbf{b} \left[f(\mathbf{k}+\mathbf{b}) - f(\mathbf{k}) \right] \;\; .$$

b) we need to express the positions of the Wannier functions and their spread as a function of the phase relations between the Bloch orbitals.

$$\mathbf{r}_n = \langle\, w_{n\mathbf{0}} \,|\, \mathbf{r} \,|\, w_{n\mathbf{0}} \,\rangle = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \langle\, u_{n\mathbf{k}} \,|\, i\frac{\partial}{\partial \mathbf{k}} \,|\, u_{n\mathbf{k}} \,\rangle$$

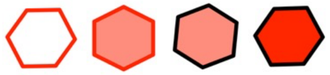


The reciprocal space representation

$$M_{mn}^{(\mathbf{k},\mathbf{b})} = \langle u_{m\mathbf{k}} \,|\, u_{n,\mathbf{k}+\mathbf{b}} \rangle$$

$$\bar{\mathbf{r}}_n = -\frac{1}{N} \sum_{\mathbf{k},\mathbf{b}} w_b \, \mathbf{b} \, \mathrm{Im} \ln M_{nn}^{(\mathbf{k},\mathbf{b})}$$

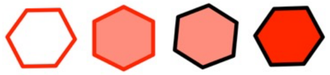
$$\langle r^2 \rangle_n = \frac{1}{N} \sum_{\mathbf{k},\mathbf{b}} w_b \left\{ \left[1 - |M_{nn}^{(\mathbf{k},\mathbf{b})}|^2 \right] + \left[\mathrm{Im} \ln M_{nn}^{(\mathbf{k},\mathbf{b})} \right]^2 \right\}$$



The localization procedure

We consider an infinitesimal rotation of the Bloch orbitals

$$|u_{n\mathbf{k}}\rangle \;\rightarrow\; |u_{n\mathbf{k}}\rangle + \sum_m dW^{(\mathbf{k})}_{mn} |u_{m\mathbf{k}}\rangle$$



The localization procedure

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$$|u_{n\mathbf{k}}\rangle \;\rightarrow\; |u_{n\mathbf{k}}\rangle + \sum_m dW^{(\mathbf{k})}_{mn}\,|u_{m\mathbf{k}}\rangle$$

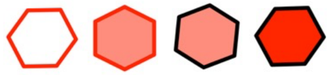
The Gradient

$$G^{(\mathbf{k})} = \frac{d\Omega}{dW^{(\mathbf{k})}} = 4\sum_{\mathbf{b}} w_b \left(\mathcal{A}[R^{(\mathbf{k},\mathbf{b})}] - \mathcal{S}[T^{(\mathbf{k},\mathbf{b})}]\right)$$

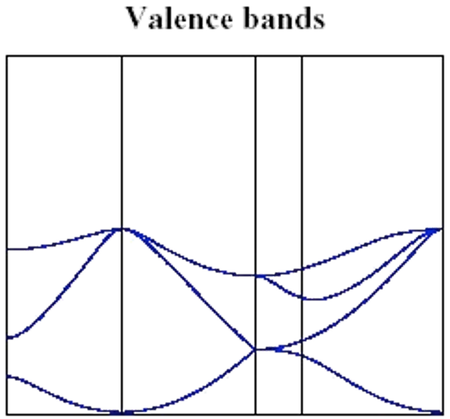
provides an equation of motion (e.g. conjugate-gradient) for the evolution of the $U^{(\mathbf{k})}_{mn}$ towards the minimum of Ω.

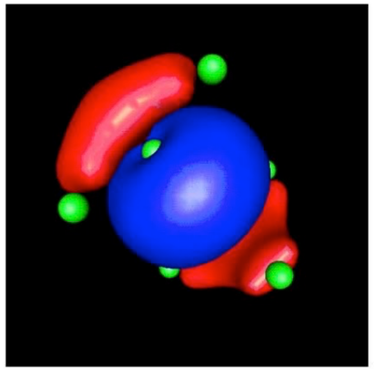
$$\mathcal{A}\,[B] = \frac{B - B^\dagger}{2} \quad , \qquad \mathcal{S}[B] = \frac{B + B^\dagger}{2i} \quad ,$$

and defining $q^{(\mathbf{k},\mathbf{b})}_n = \mathrm{Im}\,\phi^{(\mathbf{k},\mathbf{b})}_n + \mathbf{b}\cdot\mathbf{r}_n$, $T^{(\mathbf{k},\mathbf{b})}_{mn} = \widetilde{R}^{(\mathbf{k},\mathbf{b})}_{mn}\,q^{(\mathbf{k},\mathbf{b})}_n$,



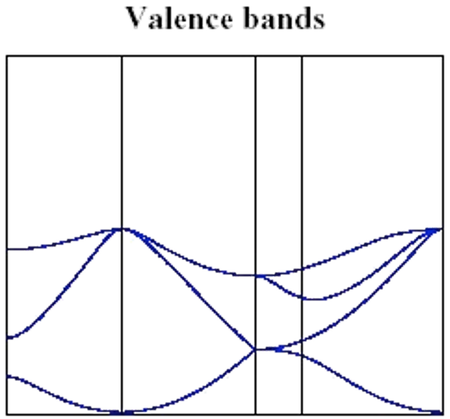
Silicon, GaAs, amorphous silicon, benzene

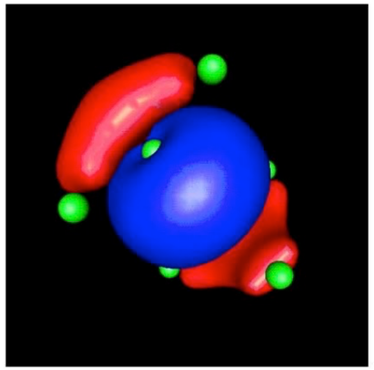


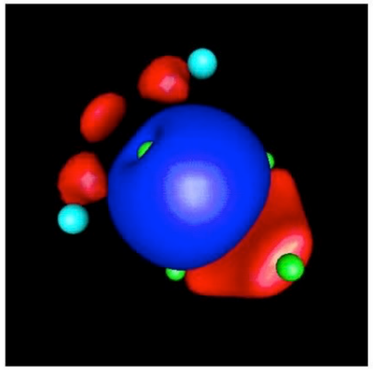


M. Fornari, N. Marzari, M. Peressi, and A. Baldereschi, Comp. Mater. Science 20, 337 (2001)

Silicon, GaAs, amorphous silicon, benzene







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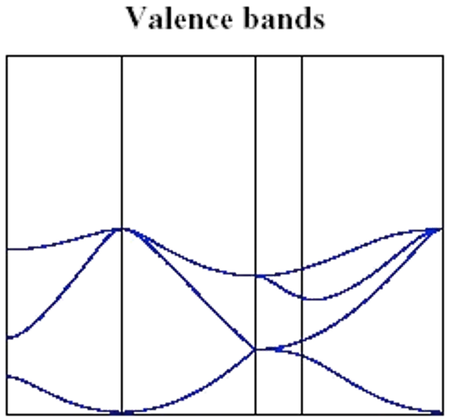

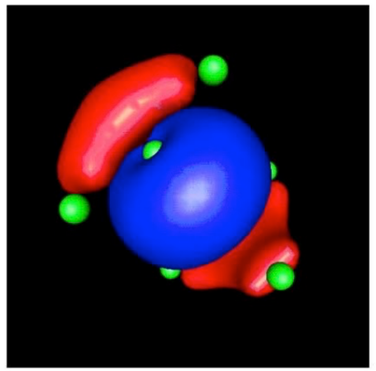

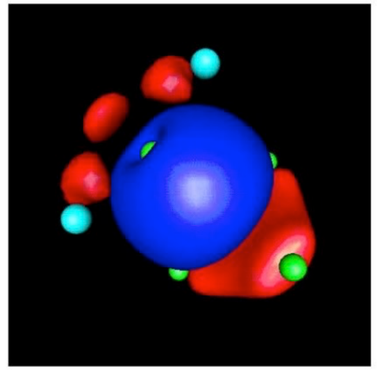

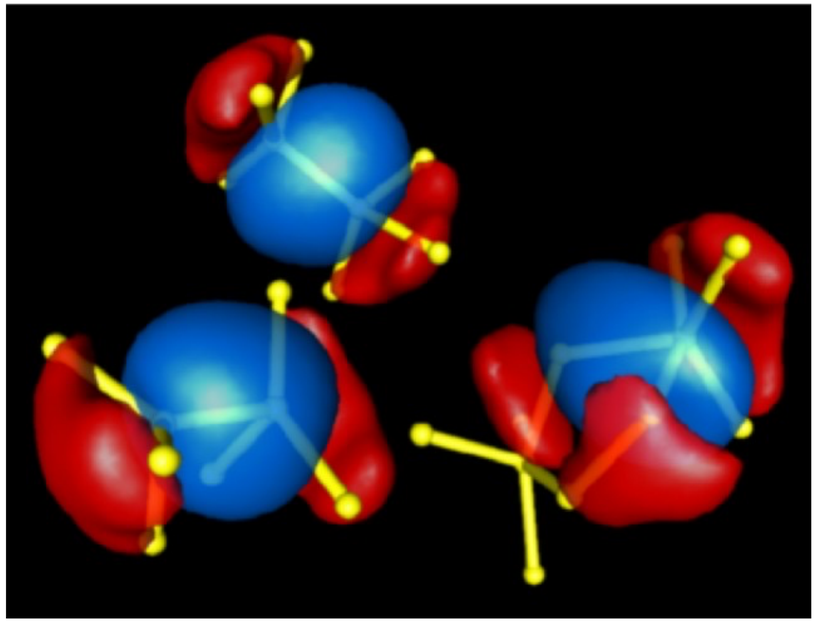

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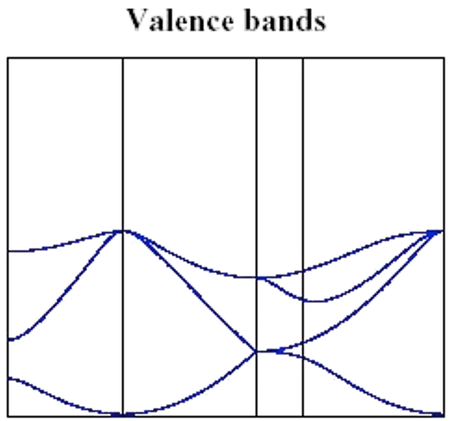
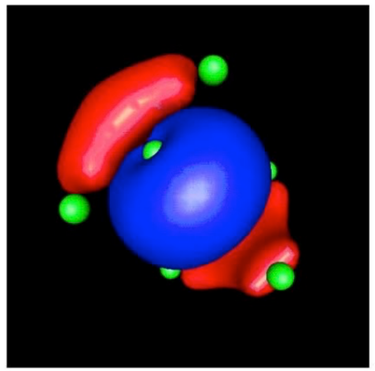
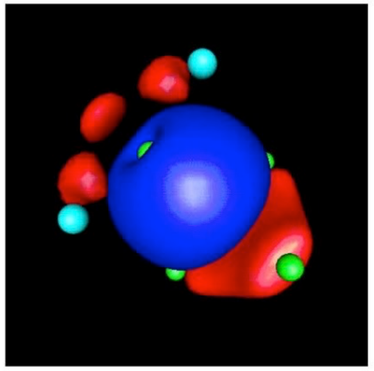
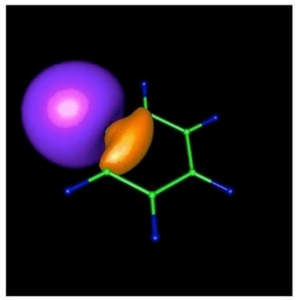
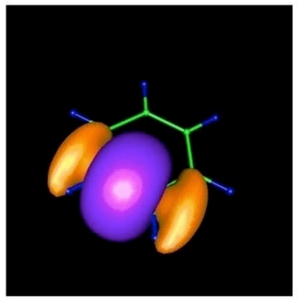
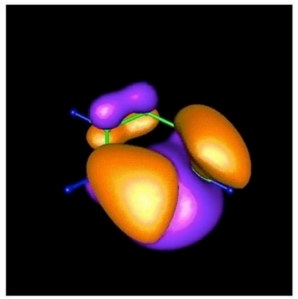


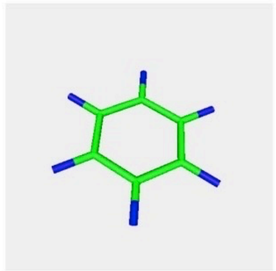


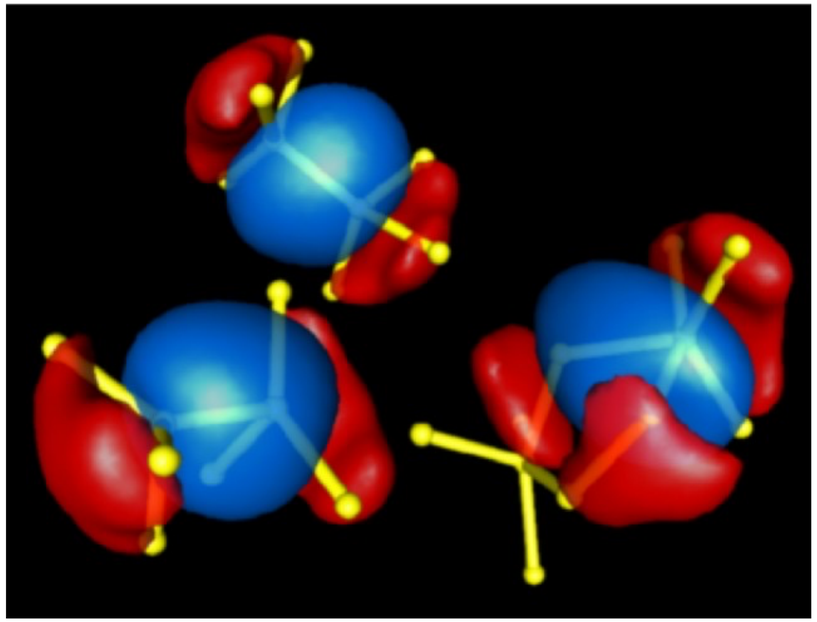








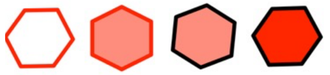




M. Fornari, N. Marzari, M. Peressi, and A. Baldereschi, Comp. Mater. Science 20, 337 (2001)

First conclusions

- general algorithm to characterize the Wannier functions (or localized orbitals) of any given system
- applicable to periodic crystals, disordered systems, isolated molecules, in the spirit of supercell calculations
- post-processing of a conventional electronic-structure calculation
- maximal localization in the orbitals obtained in the Bloch-to-Wannier transformation



What to do next?

IV. Analysis of Chemical Bonding
- A. Crystalline solids
- B. Complex and amorphous phases
- C. Defects
- D. Chemical interpretation
- E. MLWFs in first-principles molecular dynamics

V. Electric Polarization and Orbital Magnetization
- A. Wannier functions, electric polarization, and localization
  1. Relation to Berry-phase theory of polarization
  2. Insulators in finite electric field
  3. Wannier spread and localization in insulators
  4. Many-body generalizations
- B. Local polar properties and dielectric response
  1. Polar properties and dynamical charges of crystals
  2. Local dielectric response in layered systems
  3. Condensed molecular phases and solvation
- C. Magnetism and orbital currents
  1. Magnetic insulators
  2. Orbital magnetization and NMR
  3. Berry connection and curvature
  4. Topological insulators and orbital magnetoelectric response

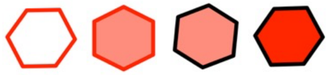
VI. Wannier Interpolation
- A. Band-structure interpolation
  1. Spin-orbit-coupled bands of bcc Fe
  2. Band structure of a metallic carbon nanotube
  3. *GW* quasiparticle bands
  4. Surface bands of topological insulators
- B. Band derivatives
- C. Berry curvature and anomalous Hall conductivity
- D. Electron-phonon coupling

VII. Wannier Functions as Basis Functions
- A. WFs as a basis for large-scale calculations
  1. WFs as electronic-structure building blocks
  2. Quantum transport
  3. Semiempirical potentials
  4. Improving system-size scaling
- B. WFs as a basis for strongly correlated systems
  1. First-principles model Hamiltonians
  2. Self-interaction and DFT + Hubbard *U*

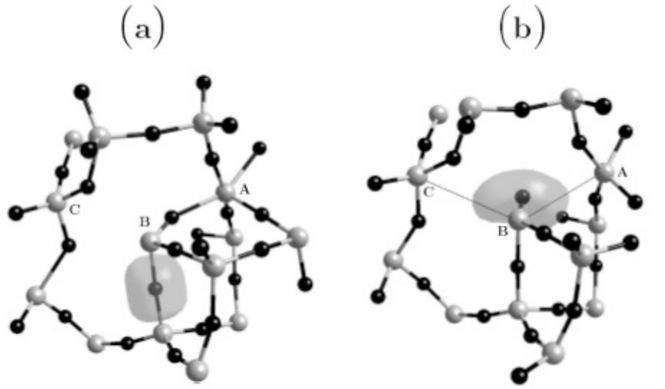
Maximally localized Wannier functions: Theory and applications

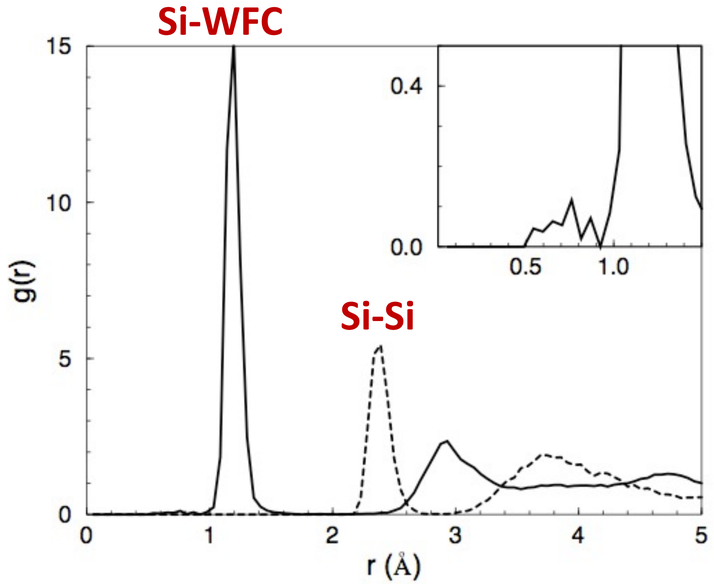
Nicola Marzari, Arash A. Mostofi, Jonathan R. Yates, Ivo Souza, David Vanderbilt

Rev. Mod. Phys. 84, 1419-1475 (2012)



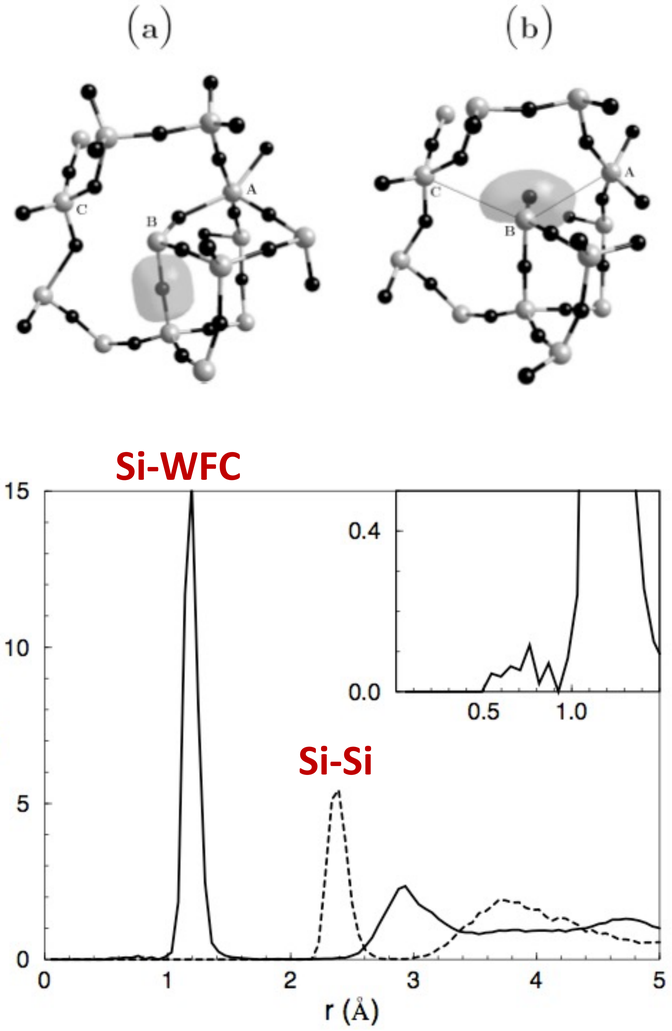
Wannier functions in *a-Si*





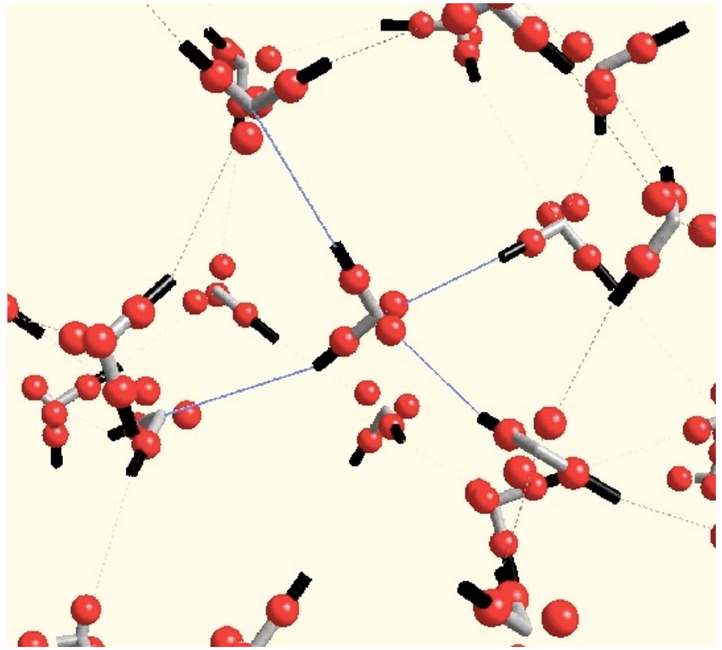
P. L. Silvestrelli, N. Marzari, D. Vanderbilt, and M. Parrinello, Solid State Comm. (1998)

Wannier functions in *a-Si*



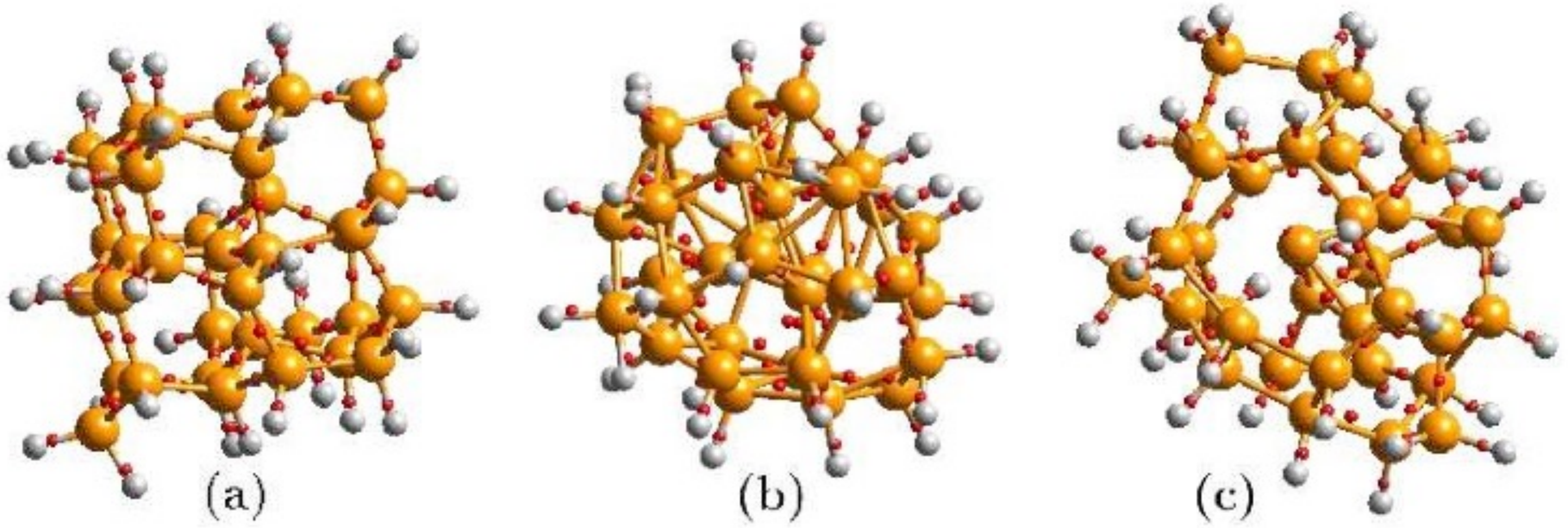
P. L. Silvestrelli, N. Marzari, D. Vanderbilt, and M. Parrinello, Solid State Comm. (1998)

Wannier functions in *l-H_2O*



P. L. Silvestrelli and M. Parrinello, JCP (1999)

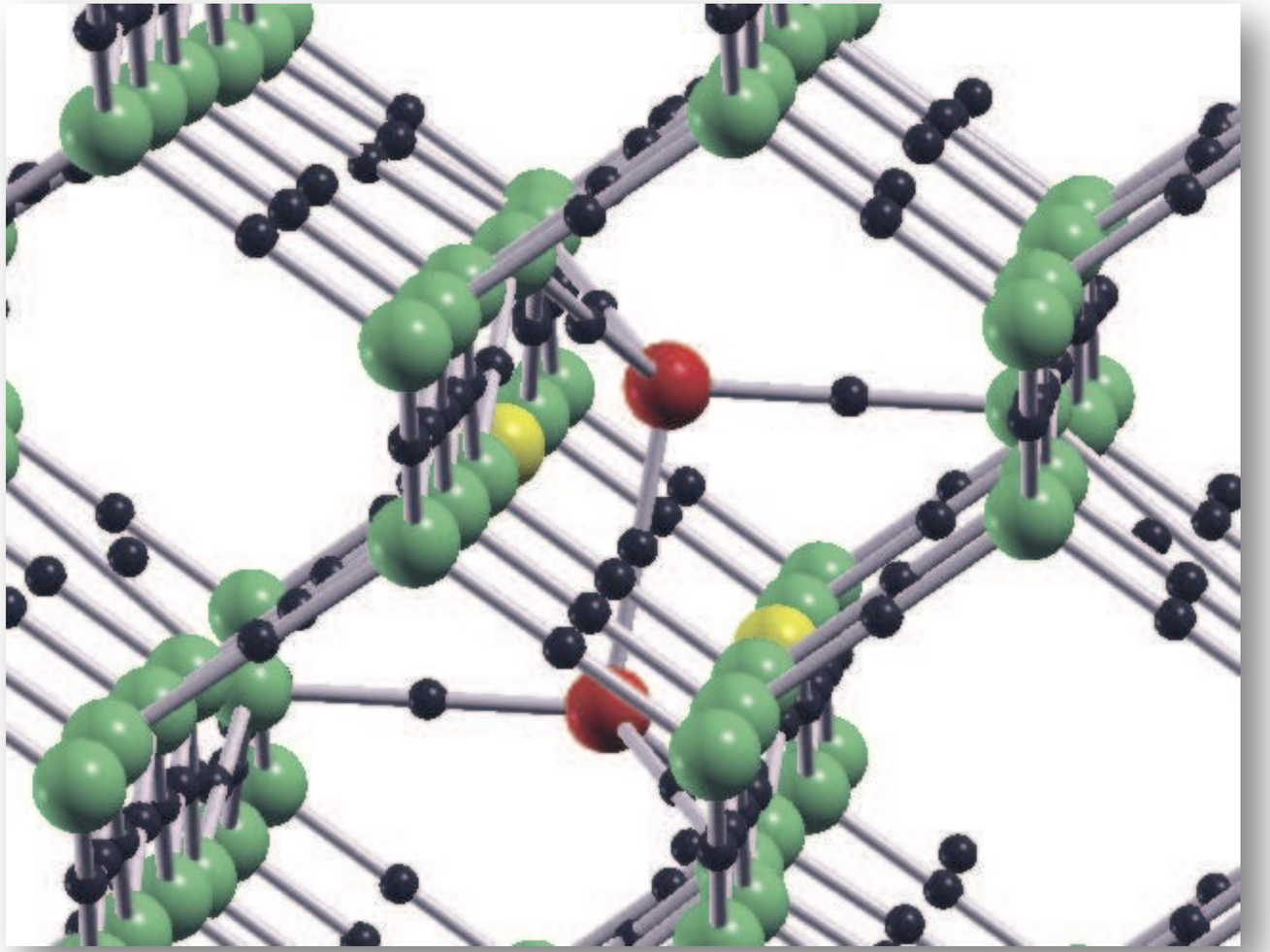
Collapse and amorphization of a Si cluster under pressure



Pressure: 25 GPa (a), 35 GPa (b) and back to 5 GPa (c).
Small red “atoms” are the Wannier centers.

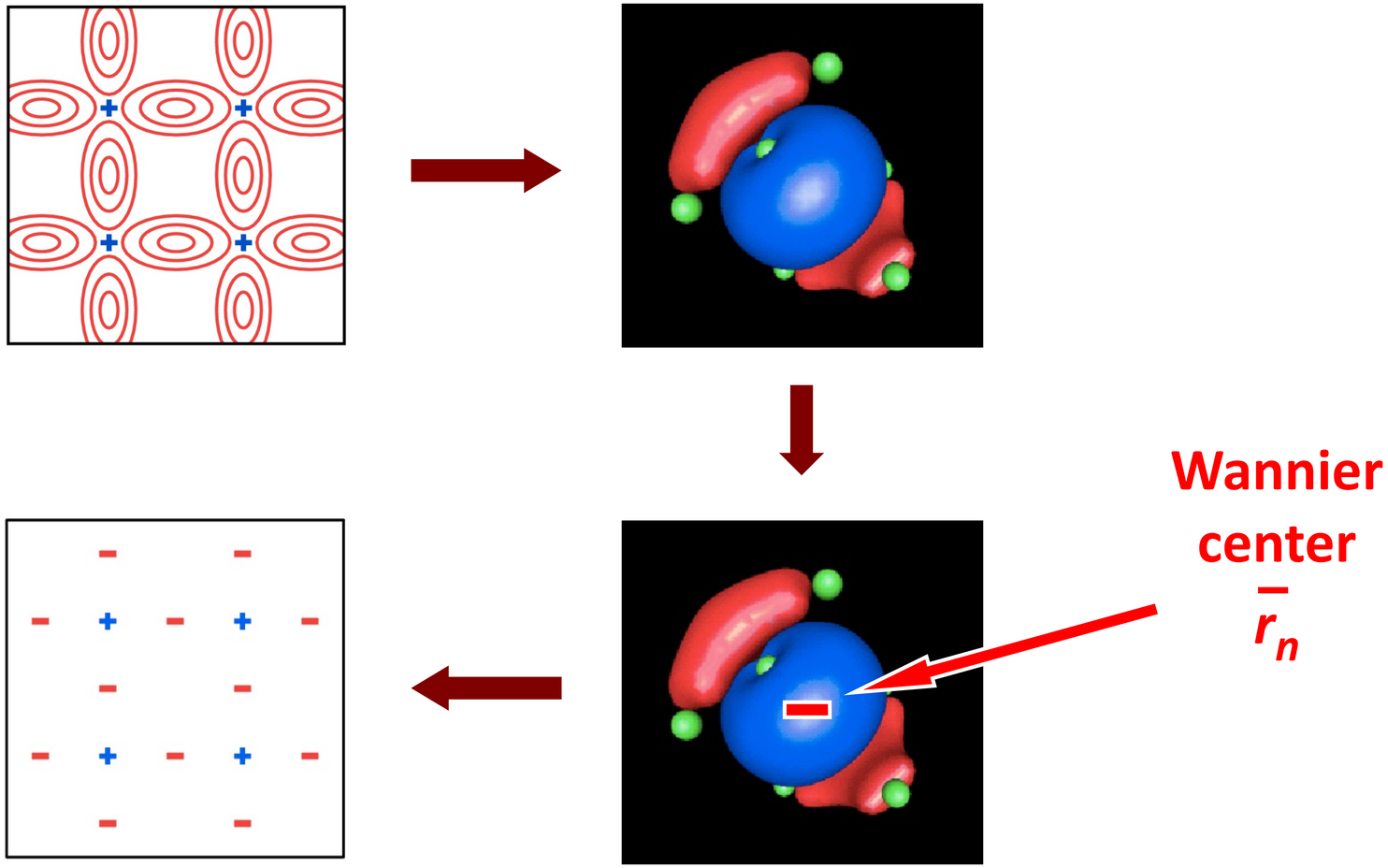
C. Molteni, R. Martoňák,, and M. Parrinello
J. Chem. Phys. 114, 5358–5365 (2001)

Fourfold coordinated defect in Si

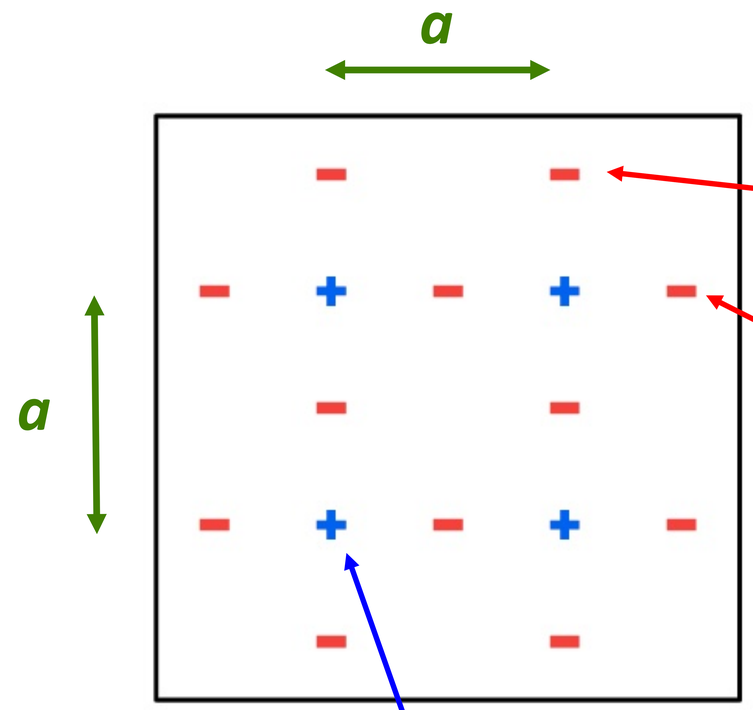


Stefan Goedecker, Thierry Deutsch, and Luc Billard,
Phys. Rev. Lett. 88, 235501 (2002)

Mapping to Wannier centers



Mapping to Wannier centers



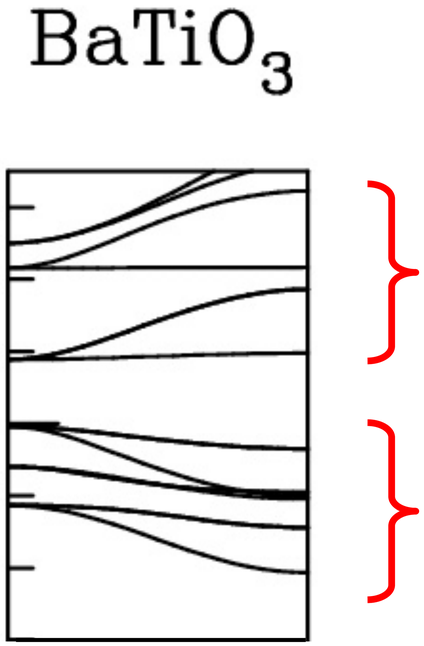
Wannier center of band 1 (charge -2e)

Wannier center of band 2 (charge -2e)

Location of ion (nucleus) (charge +4e)

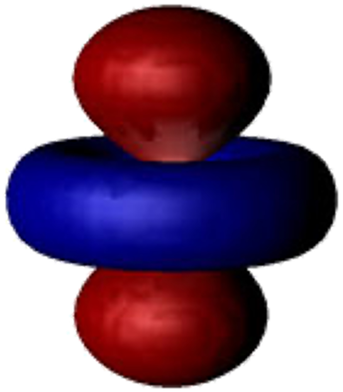
Electric polarization *P* of the crystal can be deduced from pictures like this

Wannier functions in $BaTiO_3$

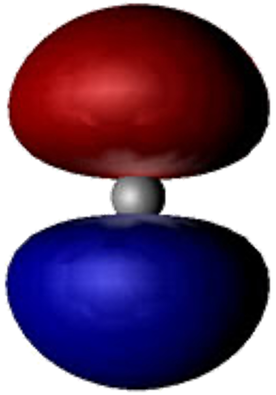


Mainly Ti *3d*
(also some O *2p*)

Mainly O *2p*
(also some Ti *3d*)



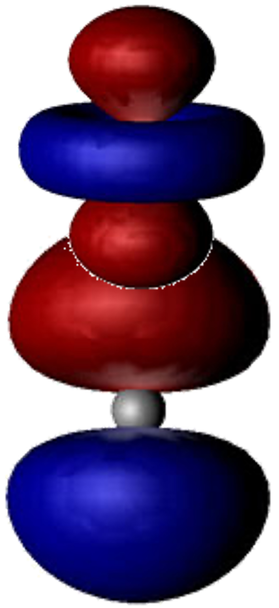
Ti *3d*



O *2p*

Example: Wannier functions in $BaTiO_3$

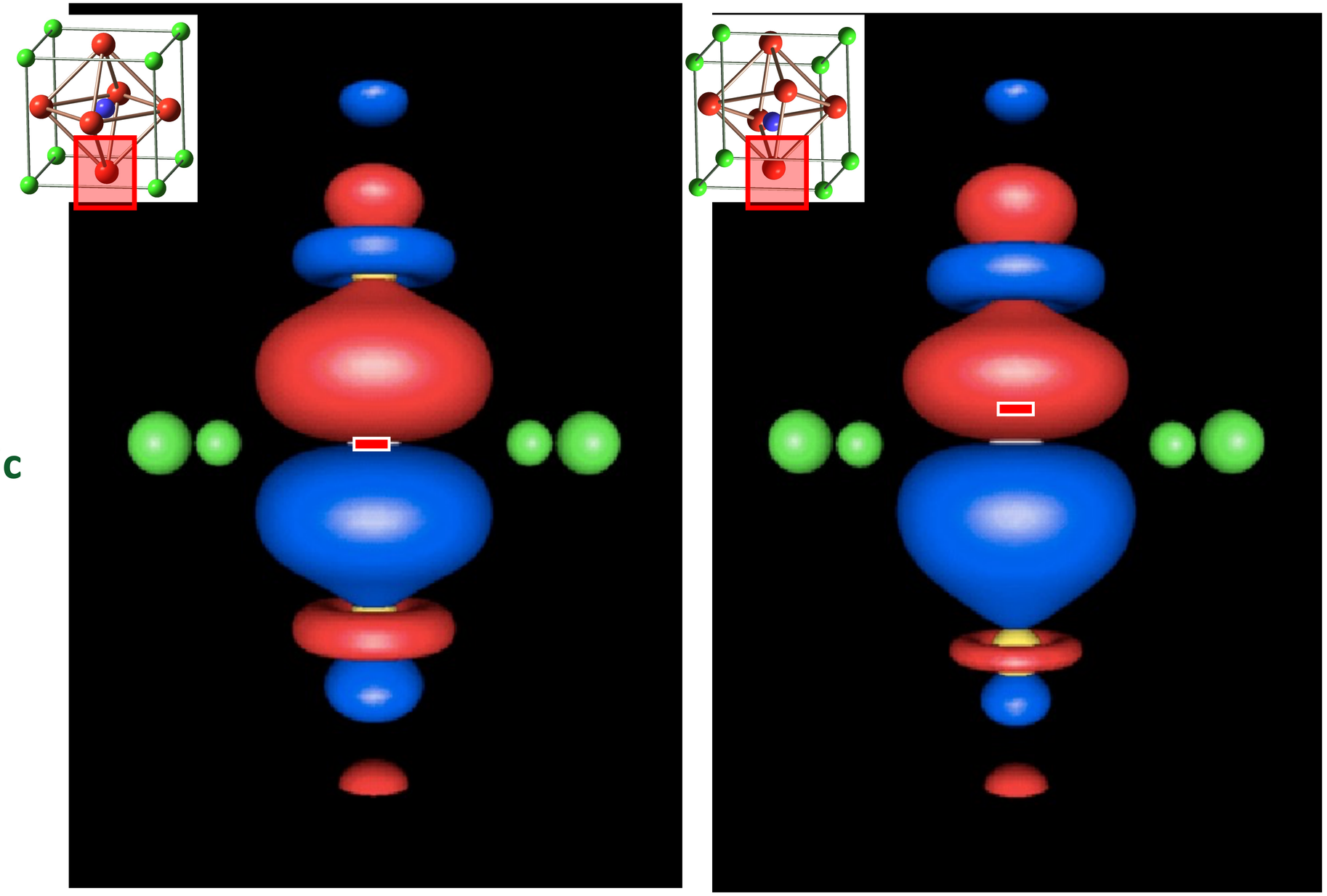
Mainly O *2p*
(also some Ti *3d*)



Ti *3d*

O *2p*

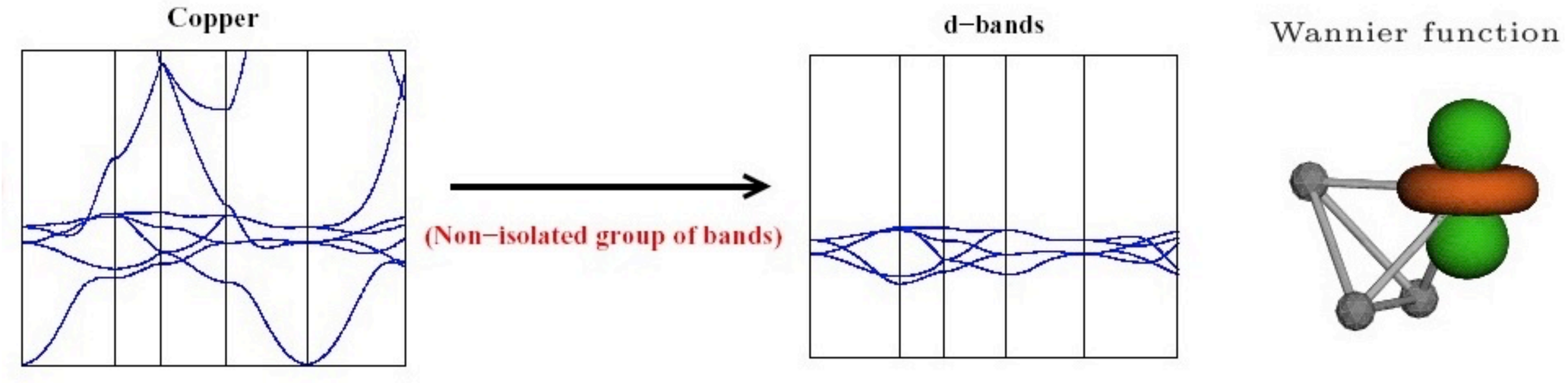
Cubic to ferroelectric $BaTiO_3$



N. Marzari and D. Vanderbilt, in *5th Williamsburg Workshop on 1st Principles Calculations for Ferroelectrics,* 146-155 (1998).

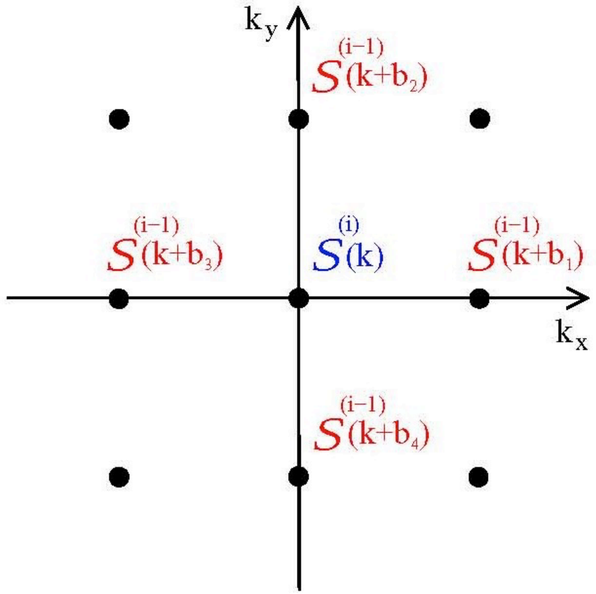
Disentanglement of attached bands

- **Maximally-localized Wannier-like functions for conduction subspace**
  - **Extract differentiable manifold with optimal smoothness**



I. Souza, N. Marzari and D. Vanderbilt, Phys. Rev. B 65, 035109 (2002)

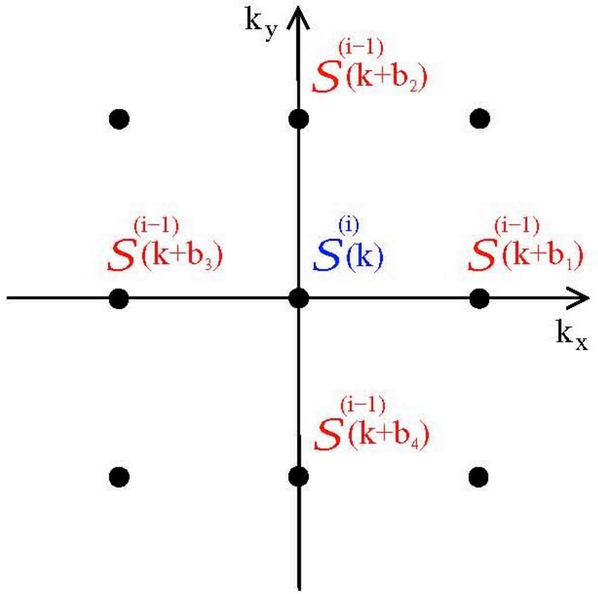
Iterative minimization of Ω_I



Minimize degree of mismatch between $\mathcal{S}^{(i)}(\mathbf{k})$ and $\mathcal{S}^{(i-1)}(\mathbf{k}+\mathbf{b})$, i.e.,

maximize overlap $\sum_{\mathbf{b}} \sum_{m=1}^{N} \left| \left\langle u_{n\mathbf{k}}^{(i)} \middle| u_{m,\mathbf{k}+\mathbf{b}}^{(i-1)} \right\rangle \right|^2$

Iterative minimization of Ω_I



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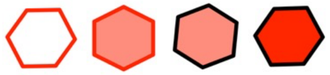
- 1^{st} iteration: Choose trial subspace at each $\mathbf{k}$ (e.g. projected orbitals)
- i^{th} iteration: At each $\mathbf{k}$ pick the N highest eigenvectors of

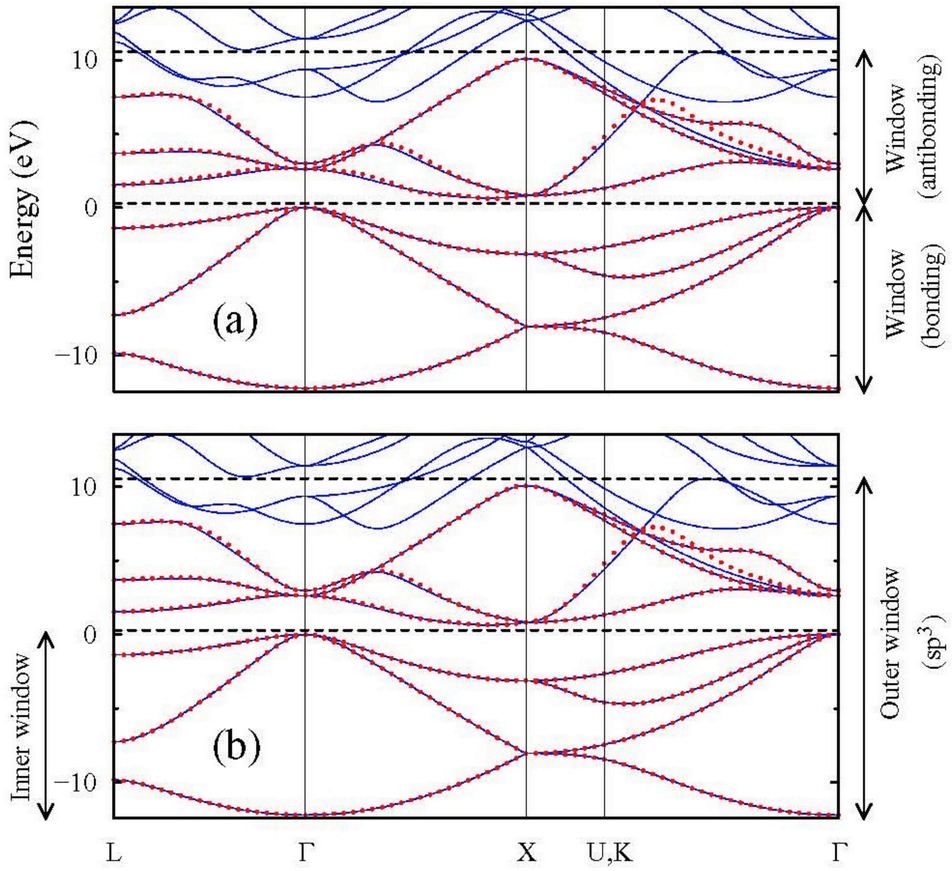
$$\left[\sum_{\mathbf{b}} \hat{P}_{\mathbf{k}+\mathbf{b}}^{(i-1)} \right] \left| u_{n\mathbf{k}}^{(i)} \right\rangle = \lambda_{n\mathbf{k}}^{(i)} \left| u_{n\mathbf{k}}^{(i)} \right\rangle$$

$\hat{P}_{\mathbf{k}+\mathbf{b}}^{(i-1)}$: Projector onto $\mathcal{S}^{(i-1)}(\mathbf{k}+\mathbf{b})$

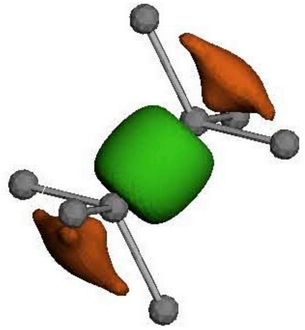
- Repeat until self-consistency (when spaces $\mathcal{S}(\mathbf{k})$ stabilize)



Silicon: bonding and antibonding orbitals

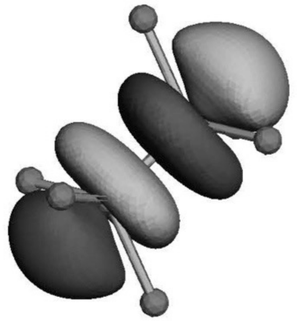


Bonding



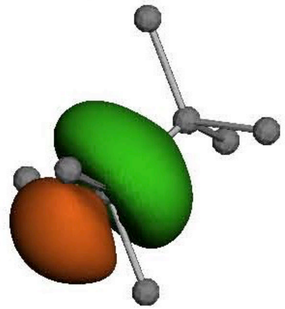
7.53 bohr^2

Antibonding



24.37 bohr^2

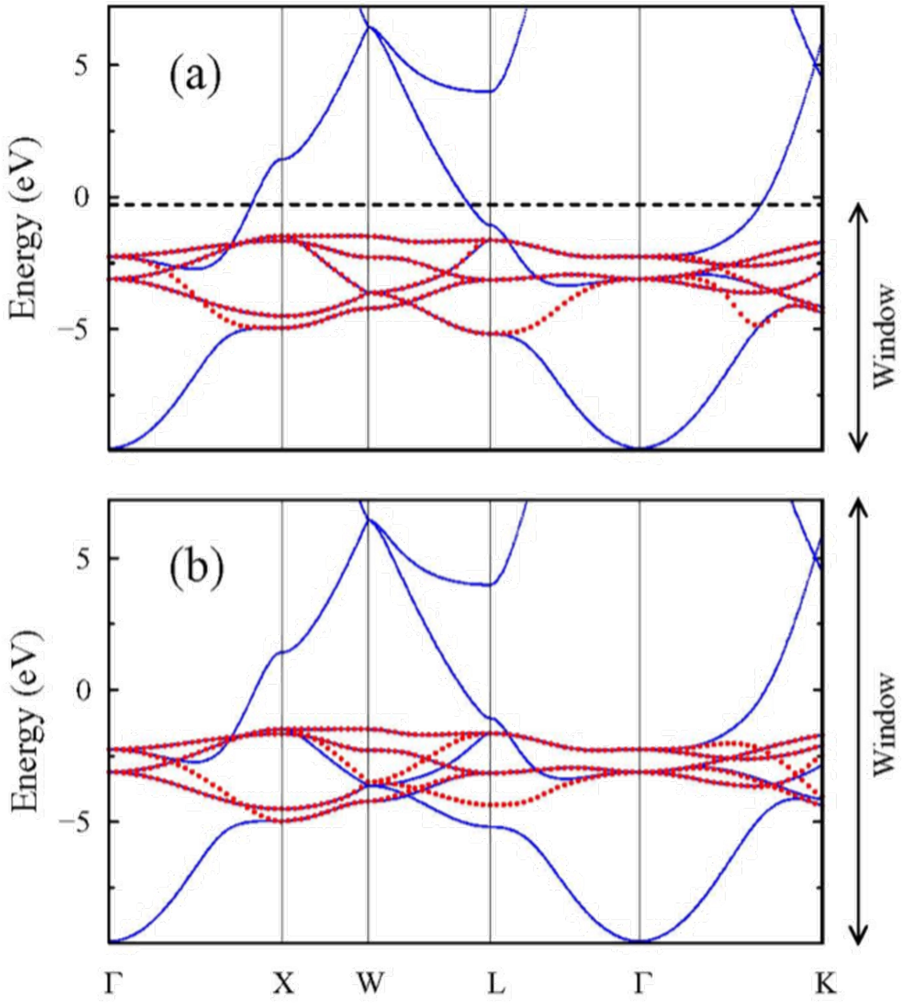
sp^3



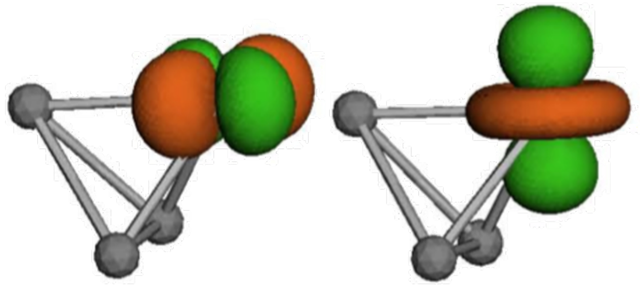
spread=10.68 bohr^2

d bands of copper

Two possible choices of energy window



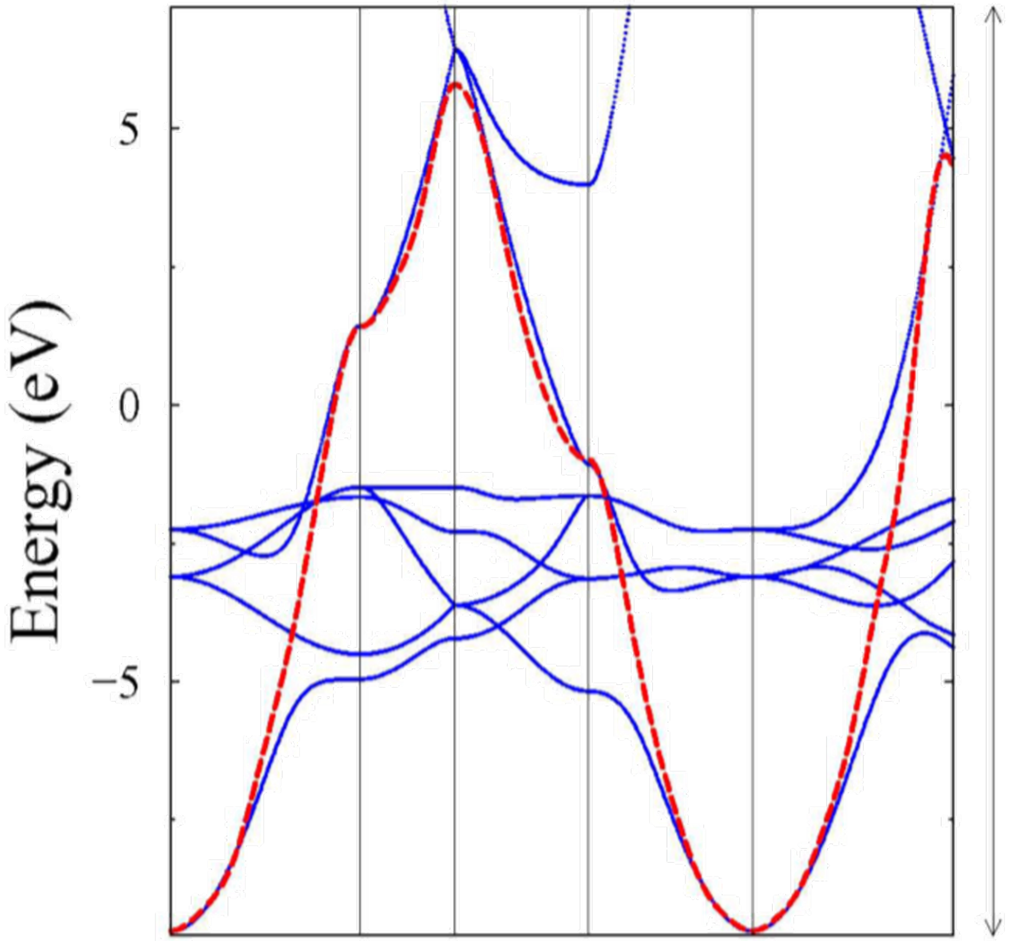
The e_g d WFs of panel (b)

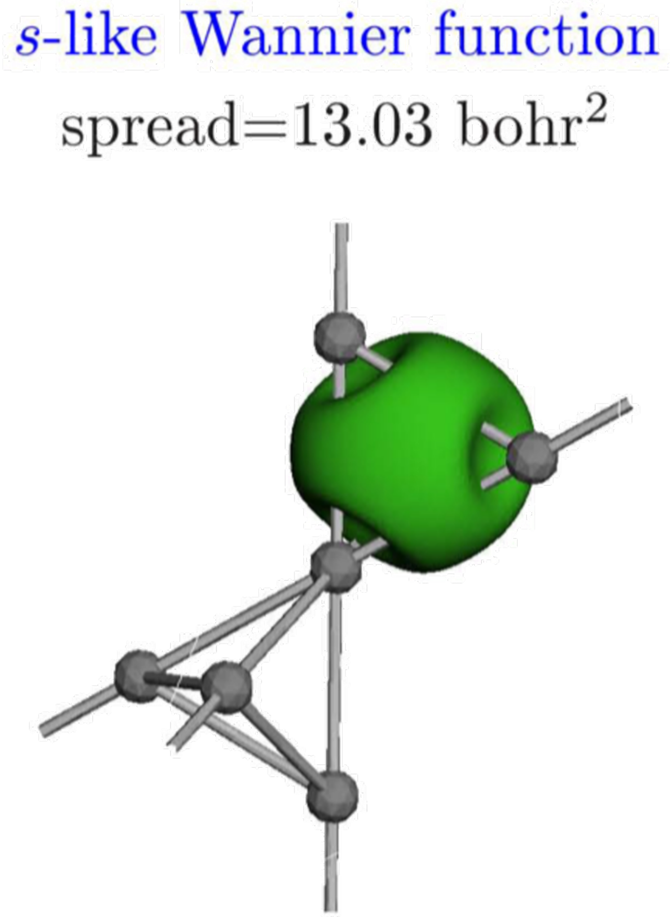


$\text{spread}(e_g)=1.700\ \text{bohr}^2$

$\text{spread}(e_g)=1.718\ \text{bohr}^2$

s band of copper

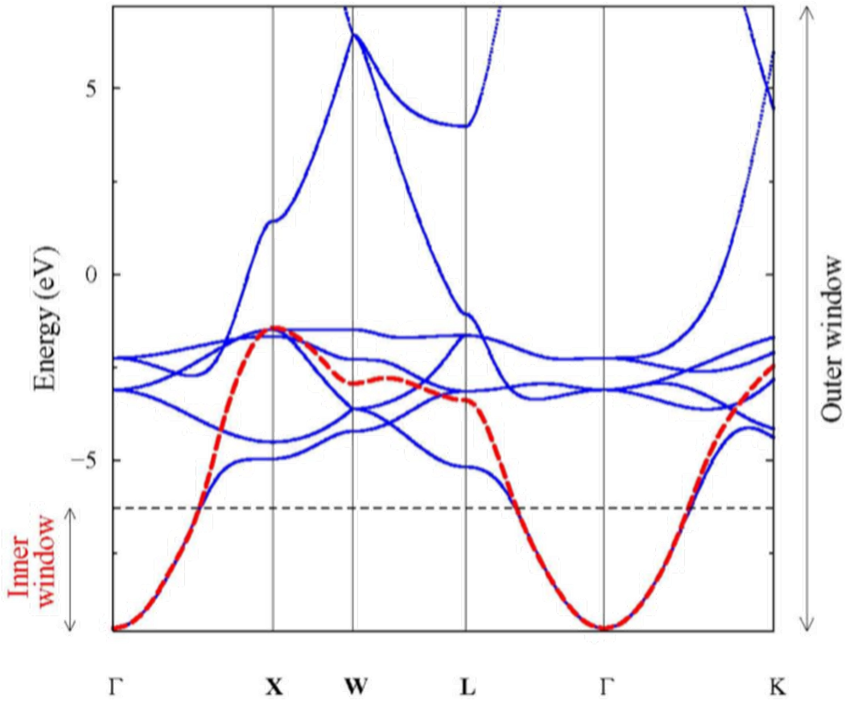




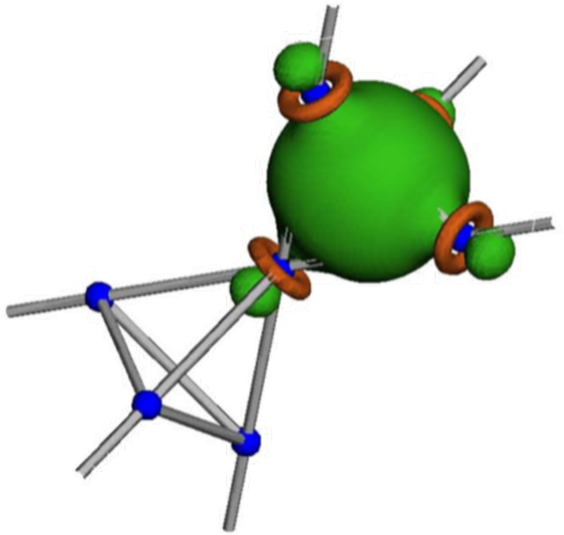
Exact constraint – frozen inner window

Suppose we want WFs to describe the original bands exactly in a prescribed energy range ("inner window").

$\Rightarrow$ Minimize Ω_{I} w/ constraint that states inside inner window are included in the optimal subspaces $\mathcal{S}(\mathbf{k})$



Hybrid *s*-*d* character:



Towards an ecosystem

PHYSICAL REVIEW B, VOLUME 65, 184422

Maximally localized Wannier functions in antiferromagnetic MnO within the FLAPW formalism

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Sandro Massidda
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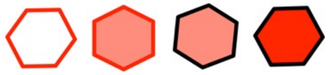
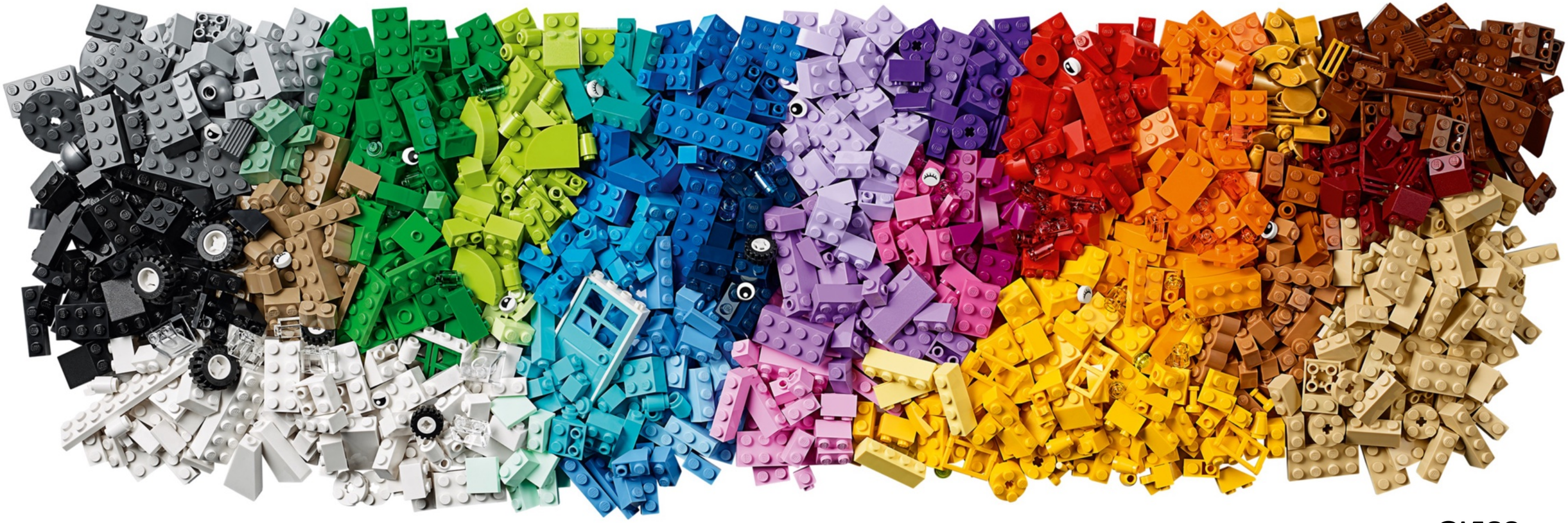
(Received 3 October 2001; published 30 April 2002)



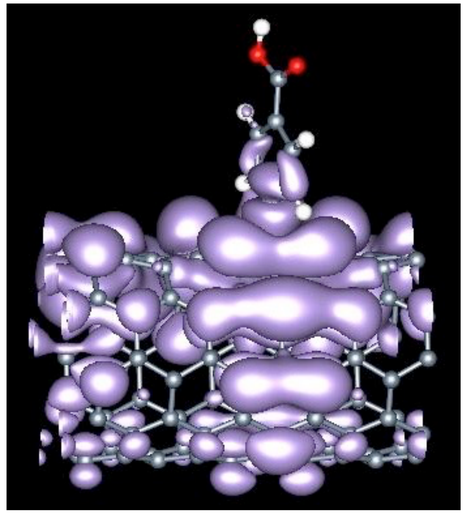
1) Bloch-by-Bloch: The LEGO bricks of electronic structure



@LEGO

Electronic structure of nanostructures

Electronic Ground State From Static or Dynamical Large-Scale Simulations → **Optimal Unitary Transformation of the Bloch Orbitals** → **Real Space Maximally-Localized Wannier Functions**

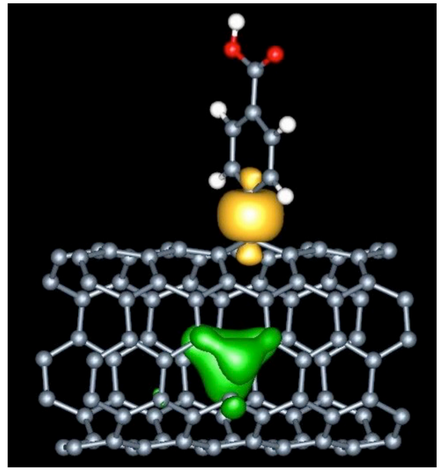


Minimization of the spread functional

$$\Omega = \sum_n [\langle r^2 \rangle_n - \langle \mathbf{r} \rangle_n^2]$$

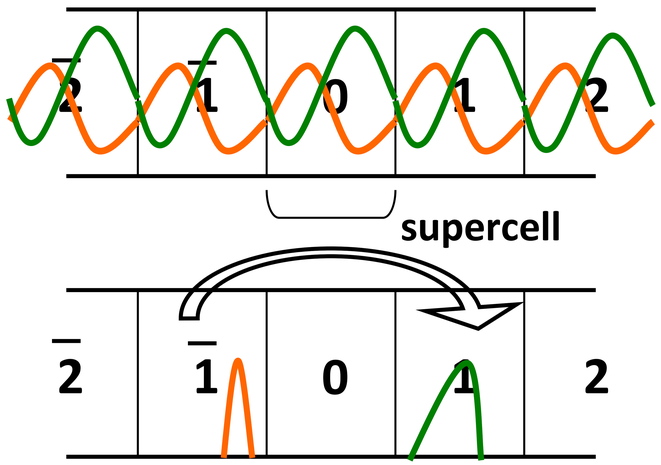
exploiting the arbitrariness of the unitary transformations between the Bloch orbitals

$$|\mathbf{R}n\rangle = \int_{BZ} \sum_m U_{mn}^{(\mathbf{k})} \Psi_{m\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$



Electronic structure of nanostructures

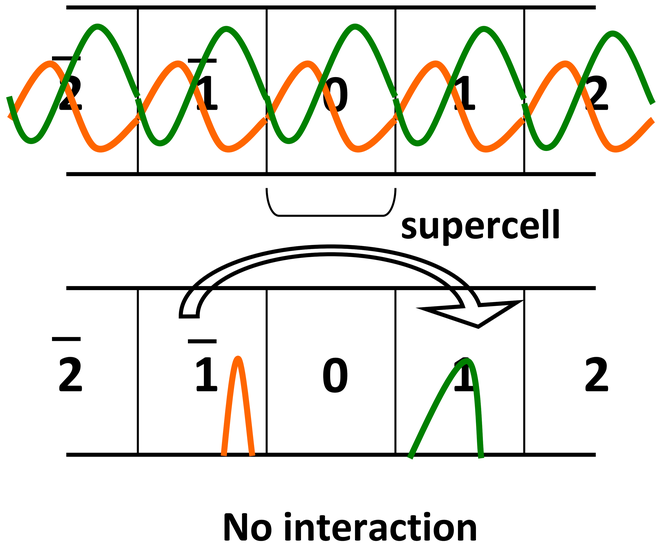
Sparse
Hamiltonian Matrix



No interaction

Electronic structure of nanostructures

Sparse Hamiltonian Matrix → **Green's Function Transmission Function**



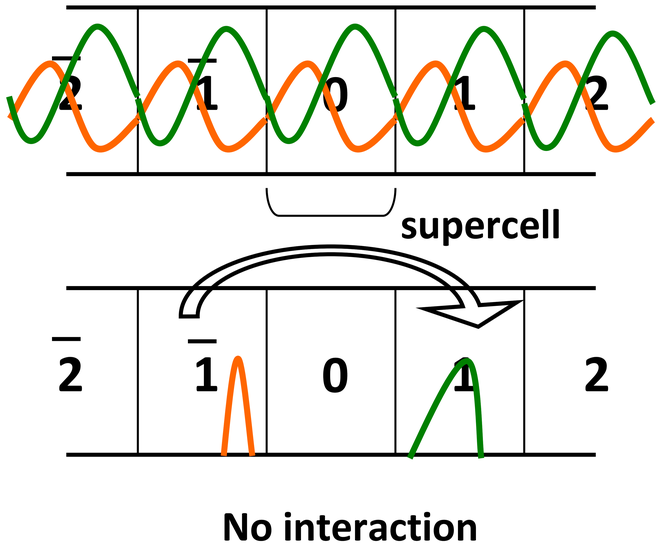
$$H_{00}\,, H_{01} \Rightarrow G_C^r(E)$$

$$T(E) = \mathrm{Tr}(\Gamma_L G_C^r \Gamma_R G_C^a)$$

$$\mathbf{H} = \begin{pmatrix} H_{01}^+ & H_{00} & H_{01} & 0 \\ & H_{01}^+ & H_{00} & H_{01} \\ & & H_{01}^+ & H_{00} & H_{01} \\ 0 & & & \end{pmatrix}$$

Electronic structure of nanostructures

Sparse Hamiltonian Matrix → **Green's Function Transmission Function** → **Ballistic Conductance Density of States**



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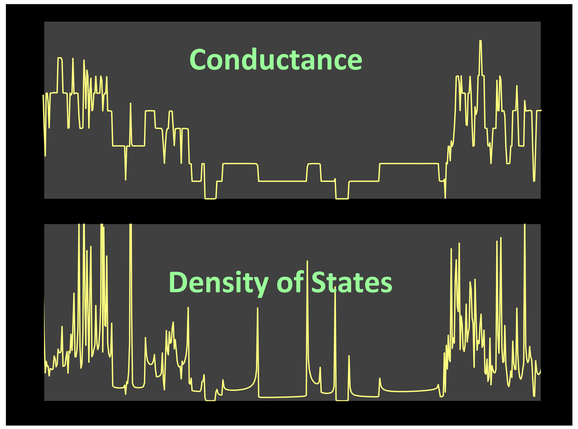
$$G(E) = \frac{2e^2}{h} T(E)$$

$$N(E) = -(1/\pi)\,\mathrm{Im}[\mathrm{Tr} G_C^r(E)]$$



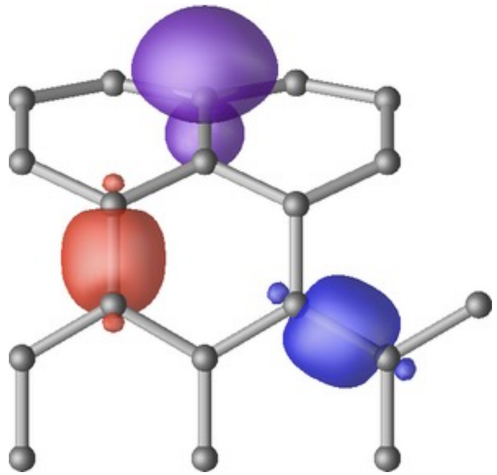
A. Calzolari, N. Marzari, I. Souza, M. B. Nardelli, Phys. Rev. B 69, 035108 (2004)

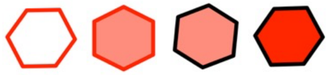
Max-loc WFs ↔ "Exact" Tight-Binding

Compact mapping of Bloch states into local orbitals

$$\omega_n(\mathbf{r}-\mathbf{R}) = \frac{V}{8\pi^3}\int_{BZ} e^{-i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r})d\mathbf{k}$$

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N_R}}\sum_R e^{i\mathbf{k}\cdot\mathbf{R}}\ \omega_n(\mathbf{r}-\mathbf{R})$$





Y.-S. Lee, M. B. Nardelli, and N. Marzari, Phys. Rev. Lett. 95, 076804 (2005)

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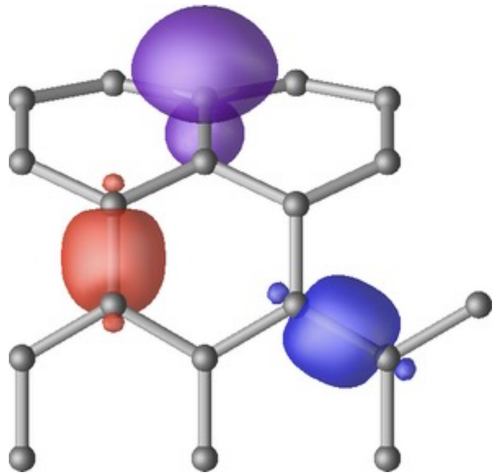
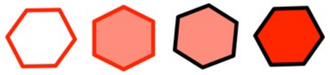


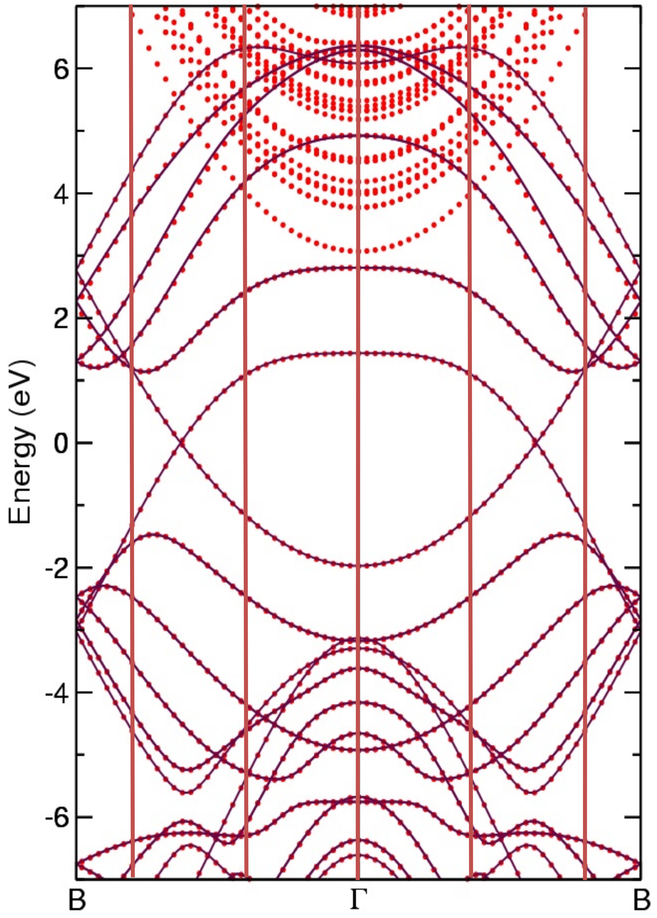
$$\left\langle \psi_{i\mathbf{k}} \middle| \hat{\mathrm{H}} \middle| \psi_{j\mathbf{k}} \right\rangle = H_{ij}^{00} + e^{i\mathbf{k}\cdot\mathbf{R}}H_{ij}^{01} + e^{-i\mathbf{k}\cdot\mathbf{R}}H_{ij}^{0\bar{1}}$$ ⇨ Diagonalize H Matrix



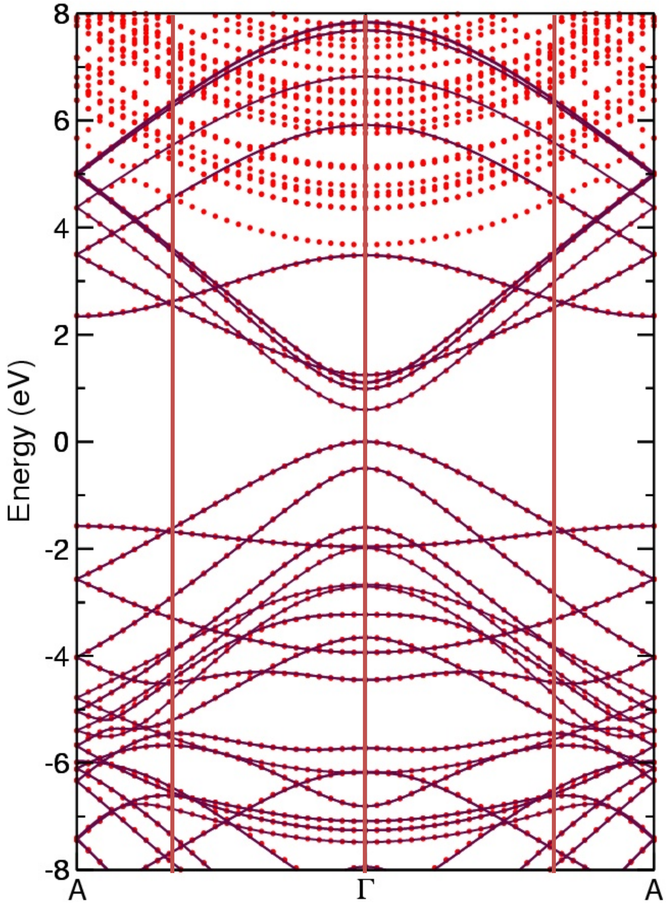
Y.-S. Lee, M. B. Nardelli, and N. Marzari, Phys. Rev. Lett. 95, 076804 (2005)

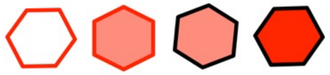
MLWFs as perfect interpolator

(5,5) SWCNT



(8,0) SWCNT





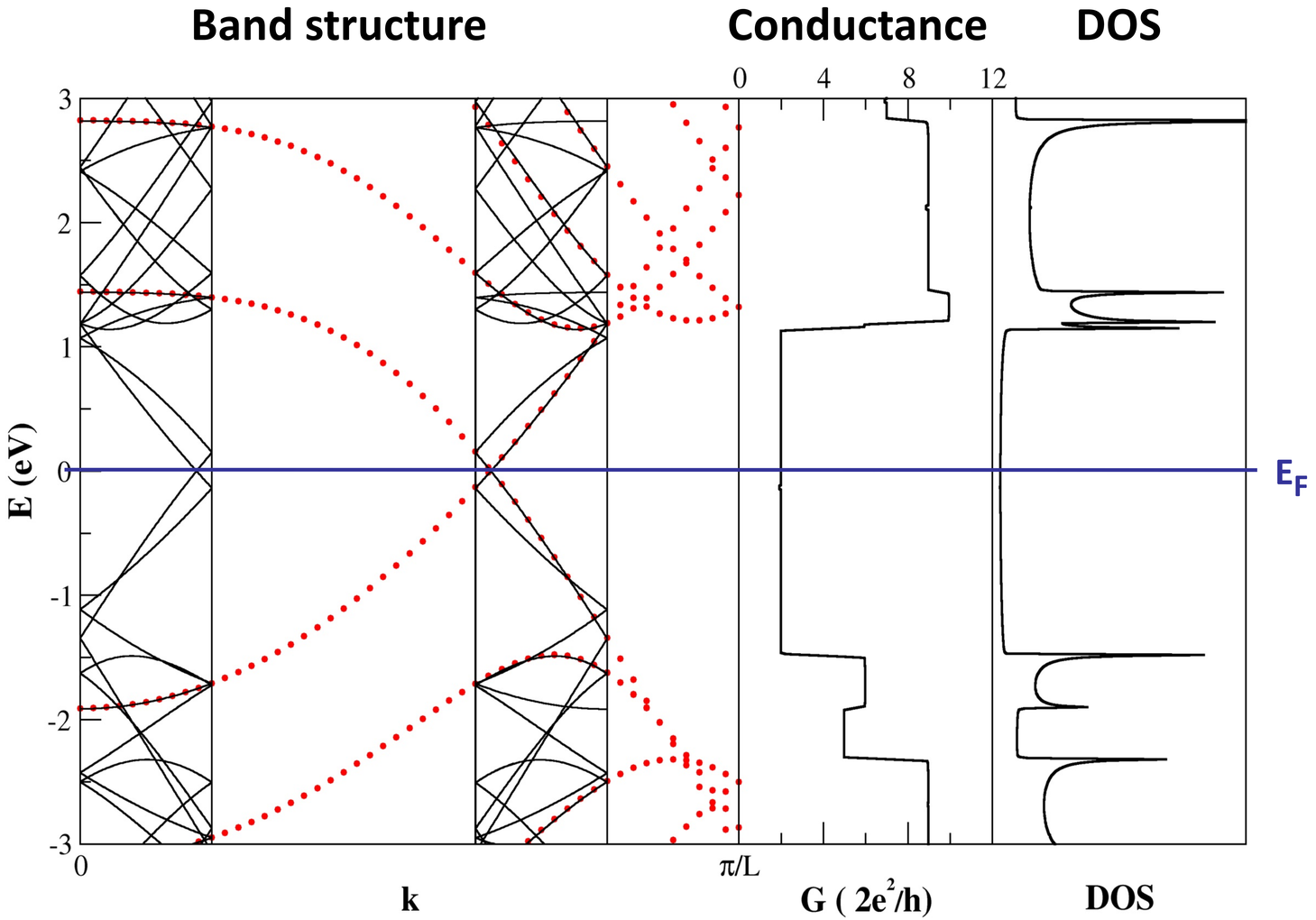
Y.-S. Lee, M. B. Nardelli, and N. Marzari, Phys. Rev. Lett. 95, 076804 (2005)

Band structure and conductance of a SWCNT

Γ-point:

2eV pseudo gap

Two eigenchannels at E_F
⇨ perfect recovery of metallic character !



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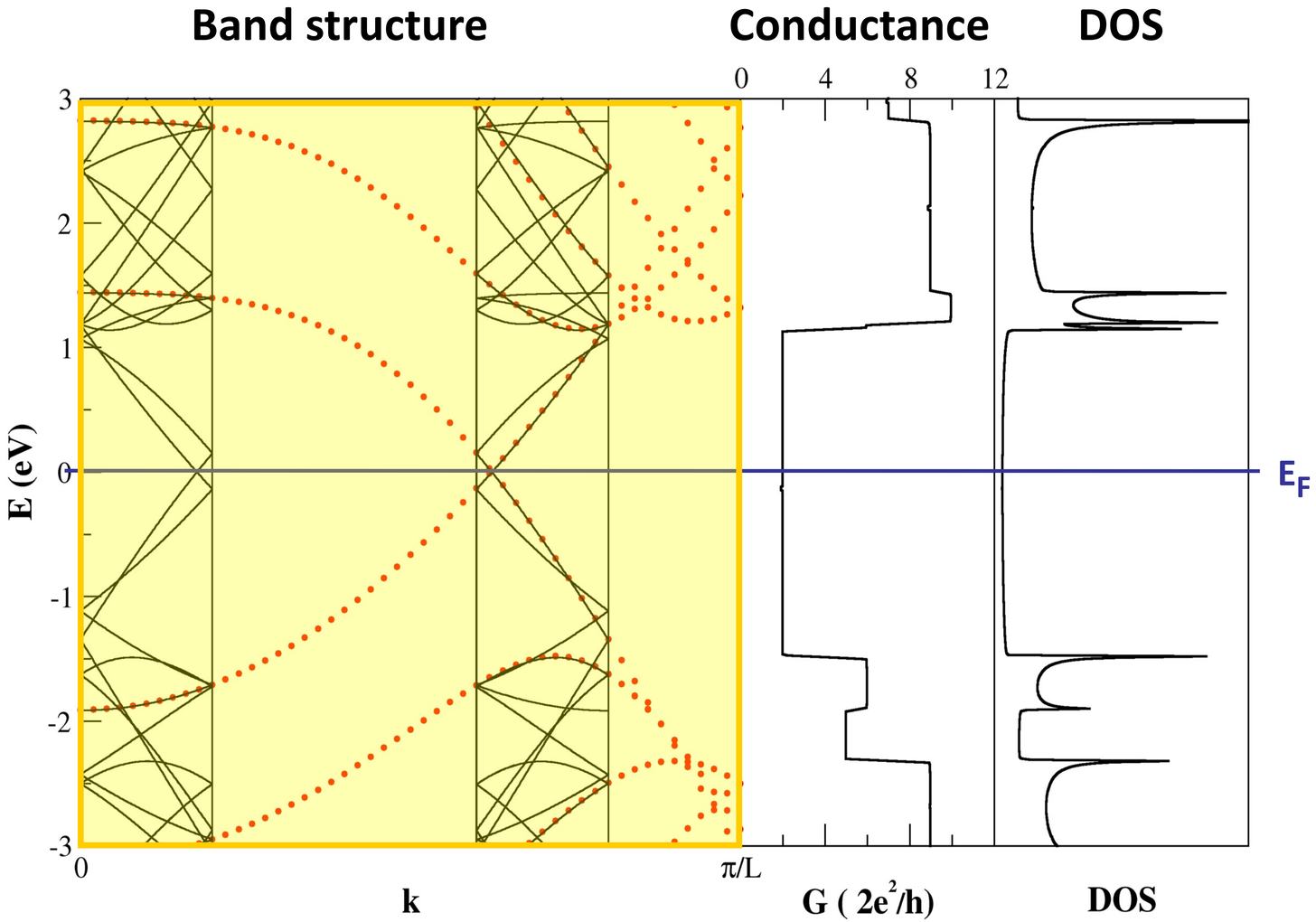

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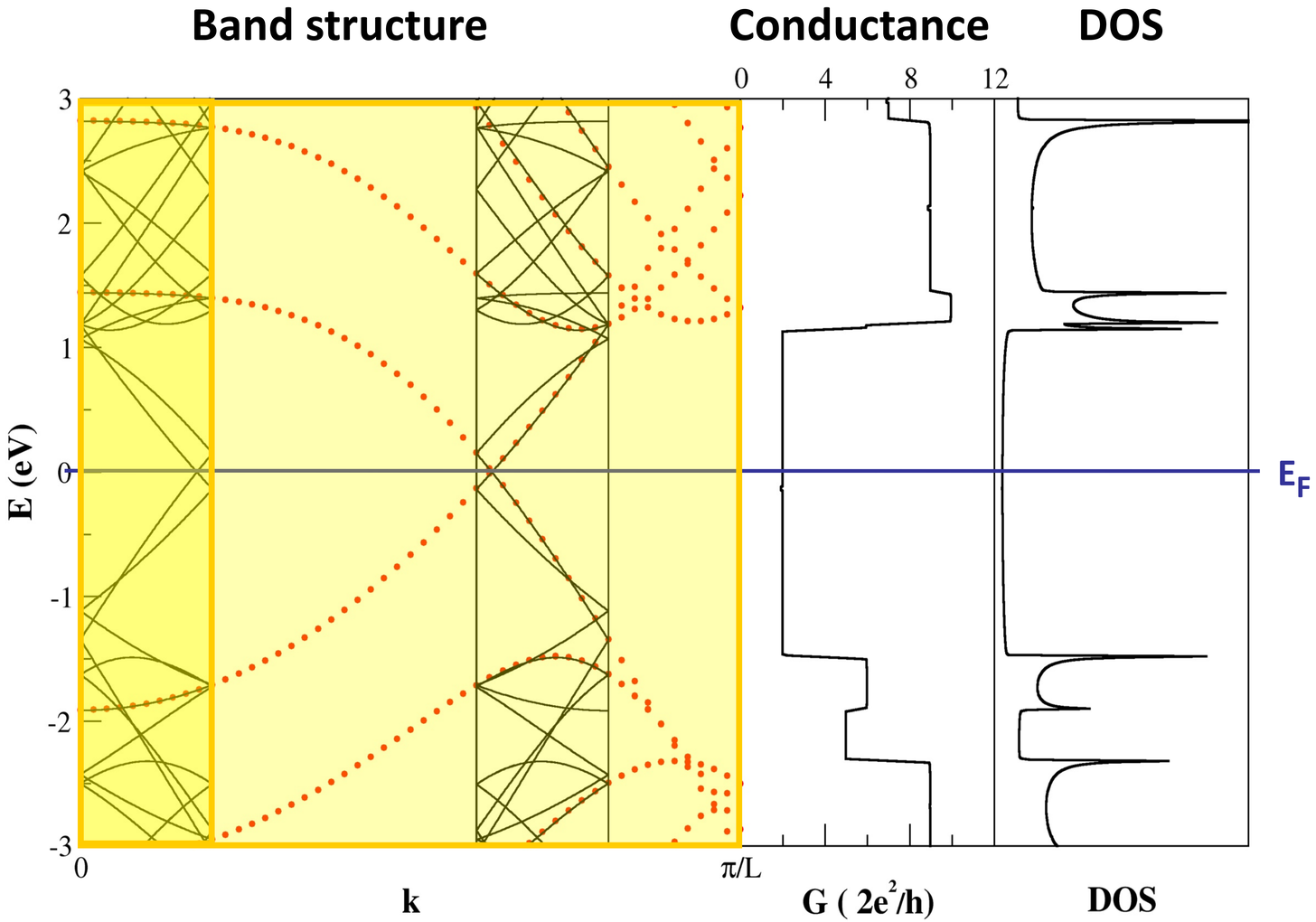

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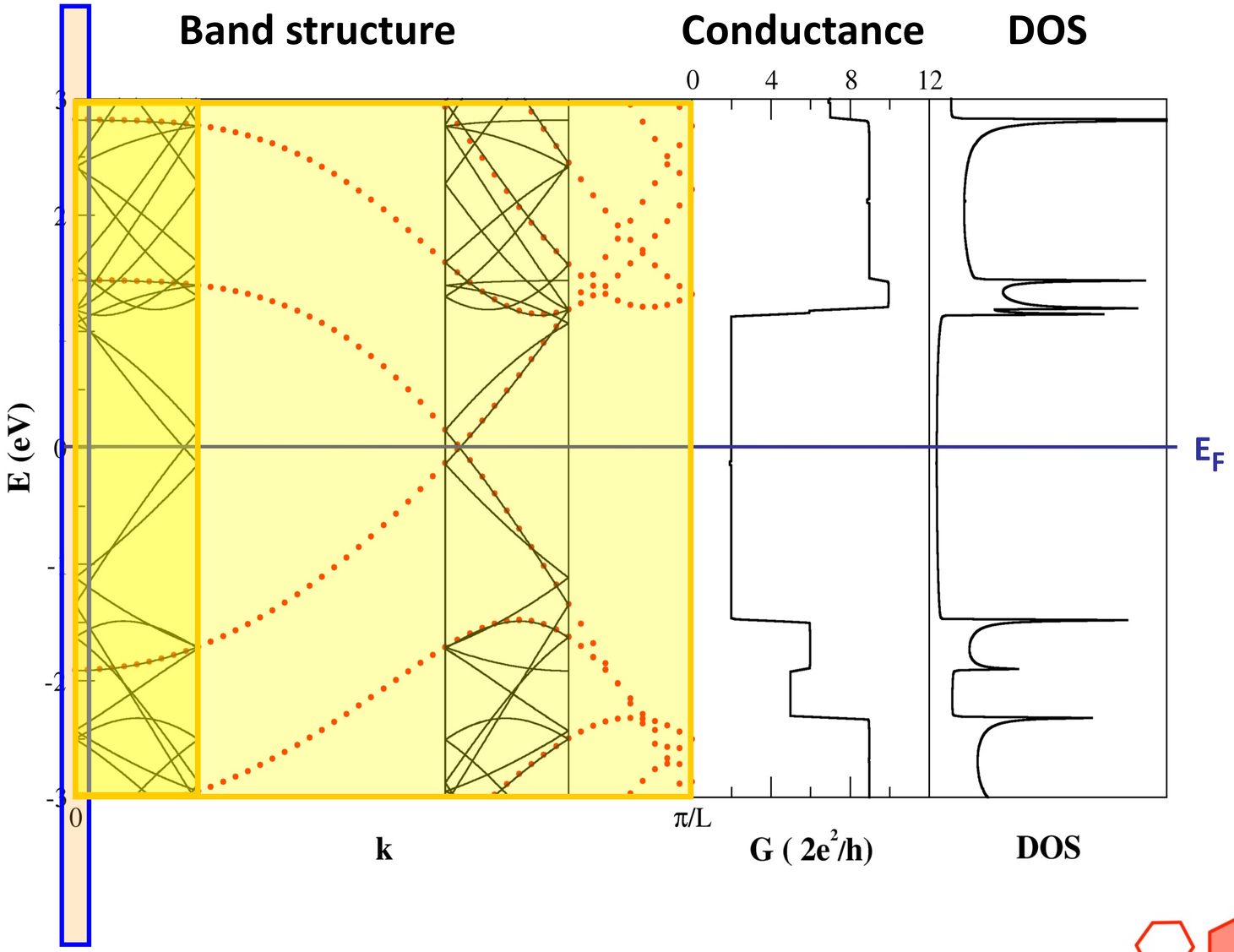


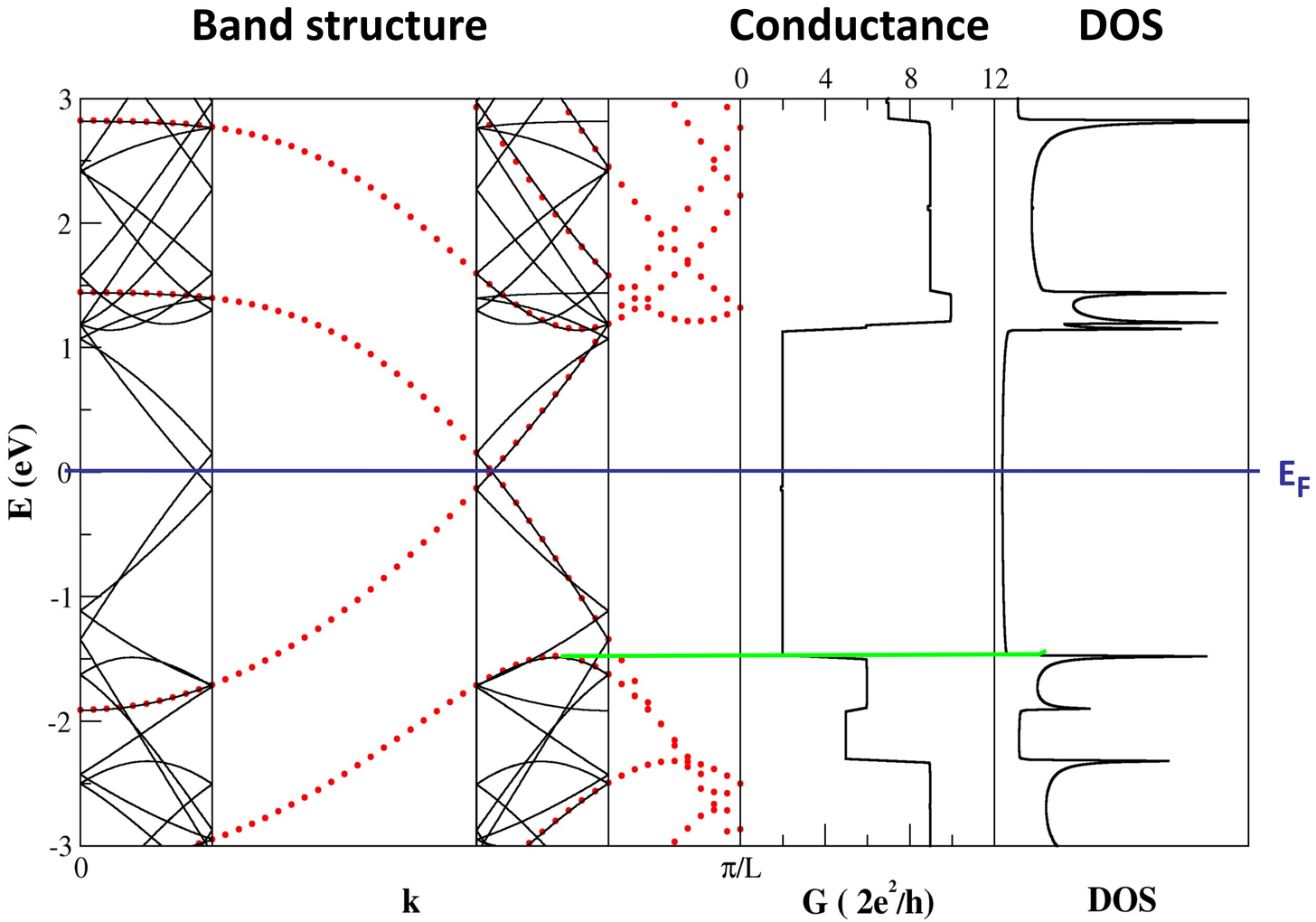
Y.-S. Lee, M. B. Nardelli, and N. Marzari, Phys. Rev. Lett. 95, 076804 (2005)

Band structure and conductance of a SWCNT

Γ-point:

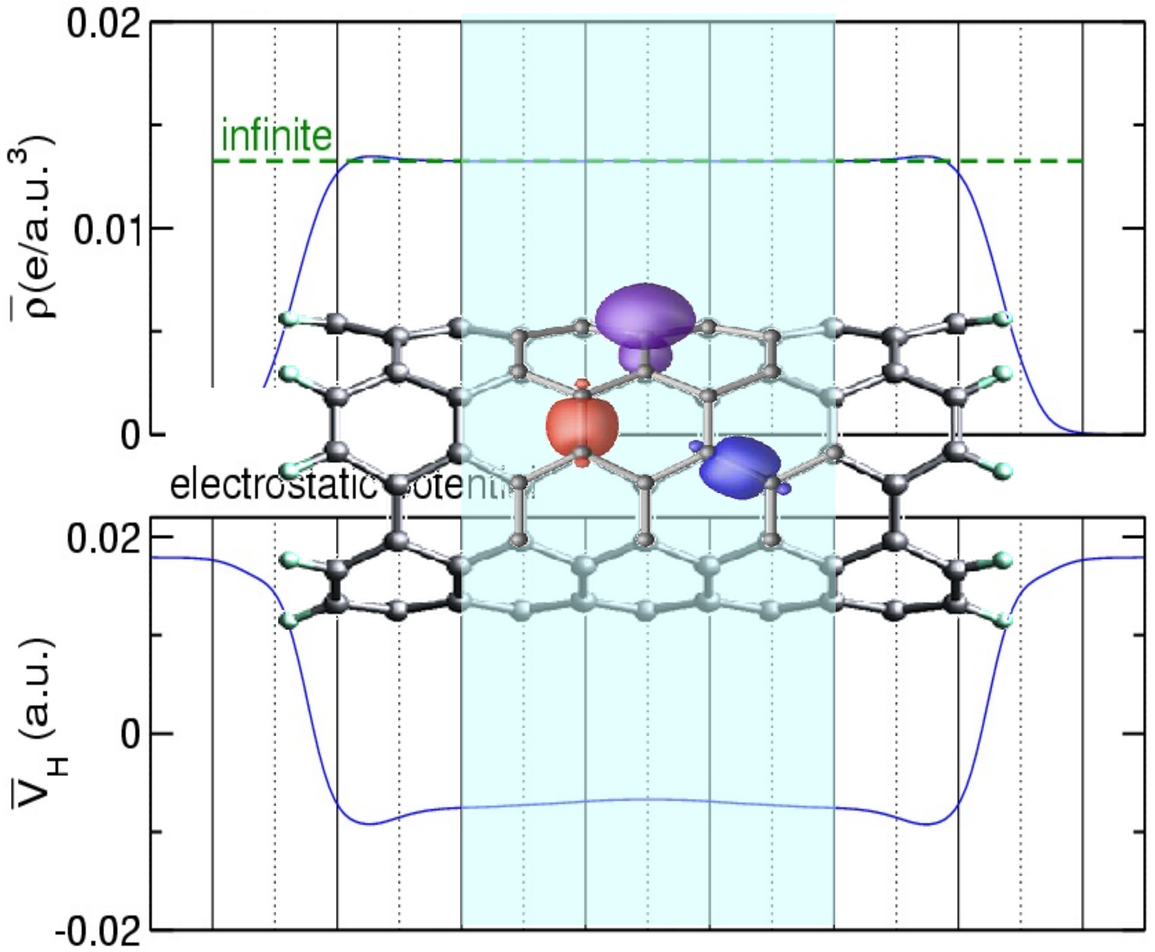
2eV pseudo gap

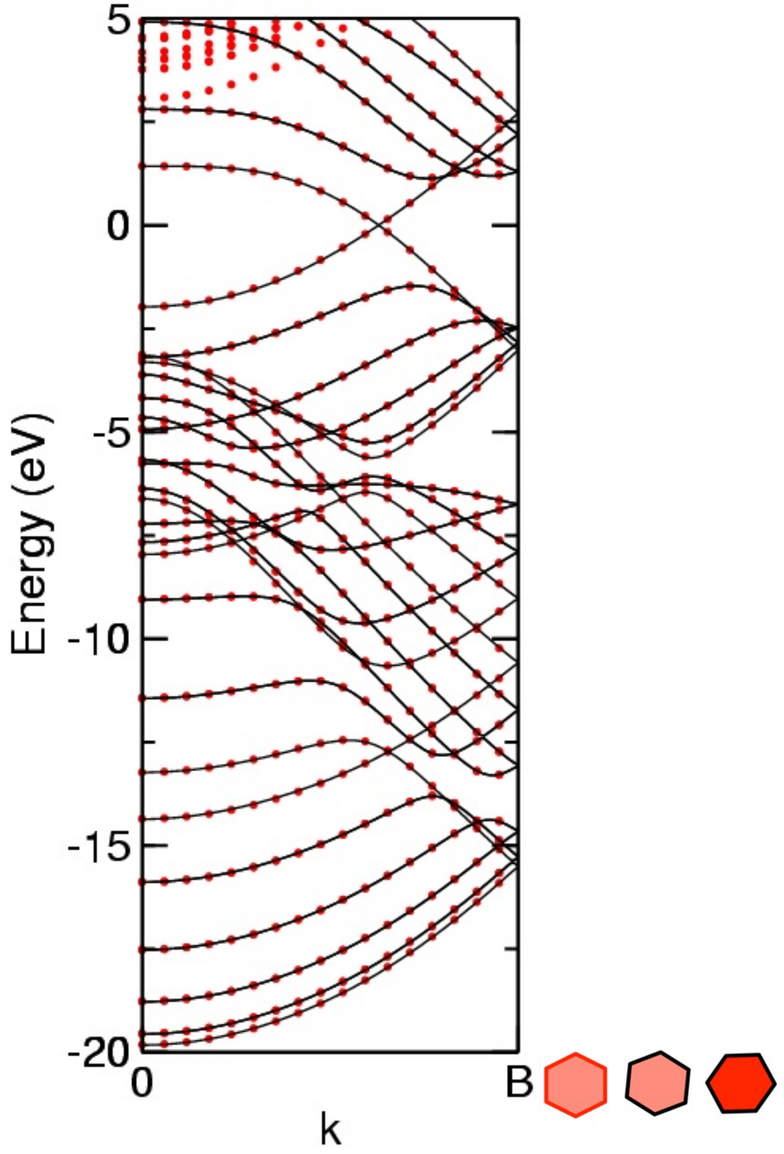
Two eigenchannels at E_F
⇨ perfect recovery of metallic character !



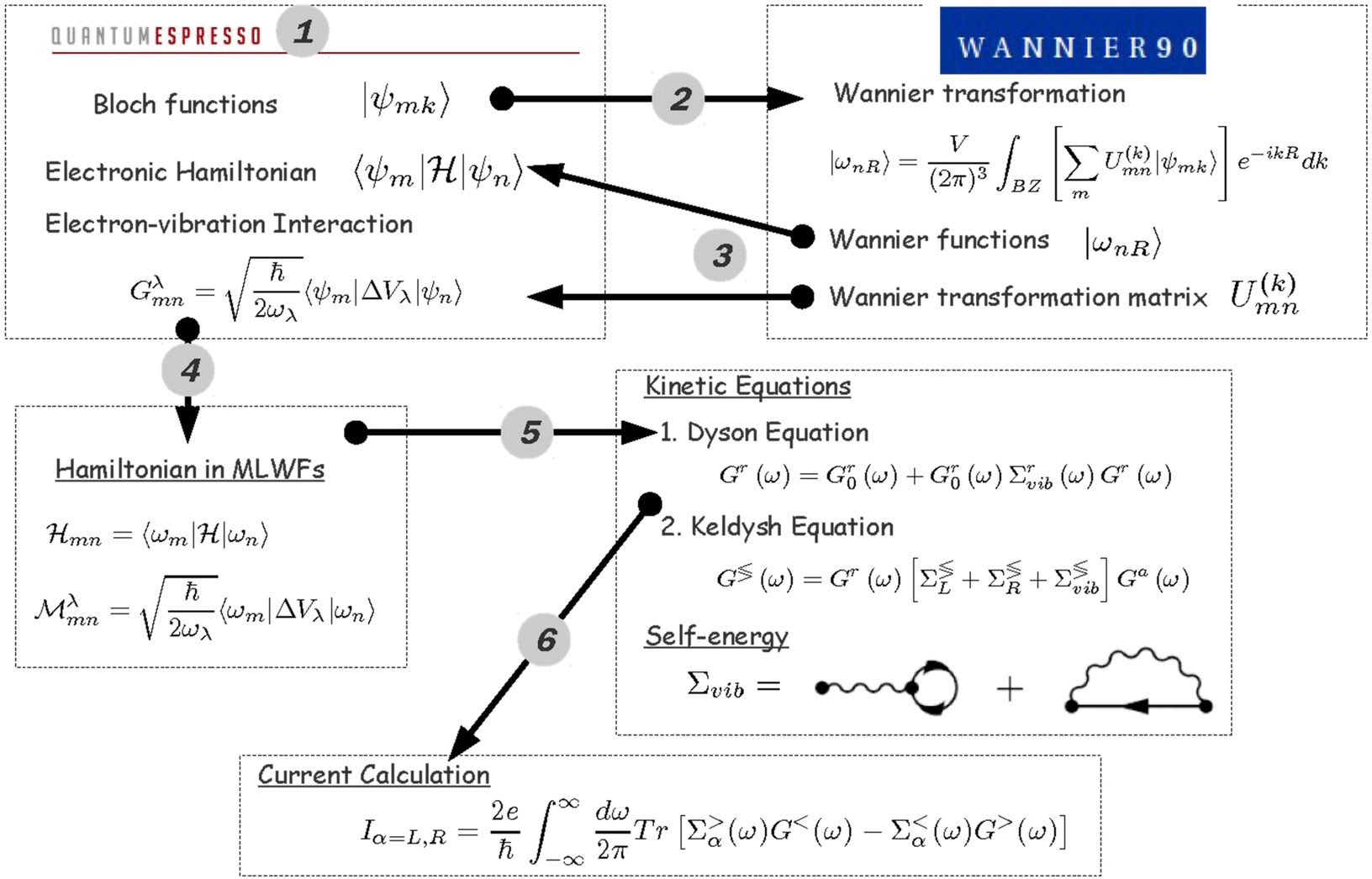
Y.-S. Lee, M. B. Nardelli, and N. Marzari, Phys. Rev. Lett. 95, 076804 (2005)

The LEGO bricks of electronic structure





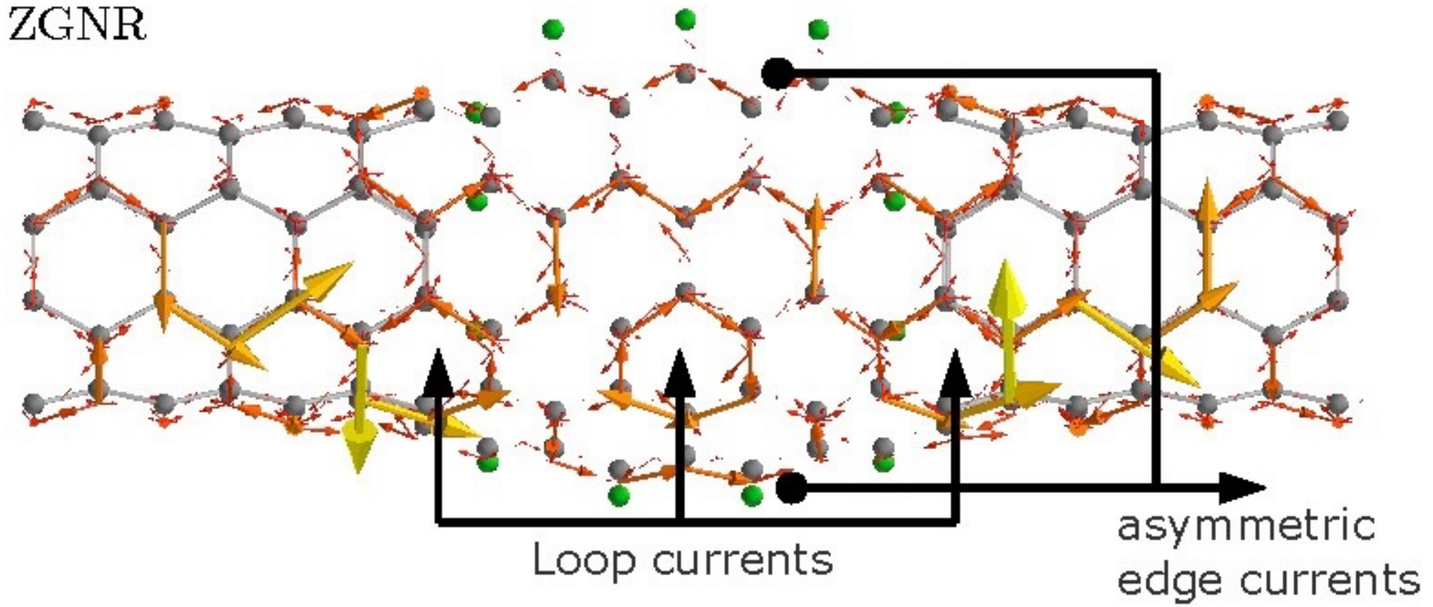
Inelastic quantum transport



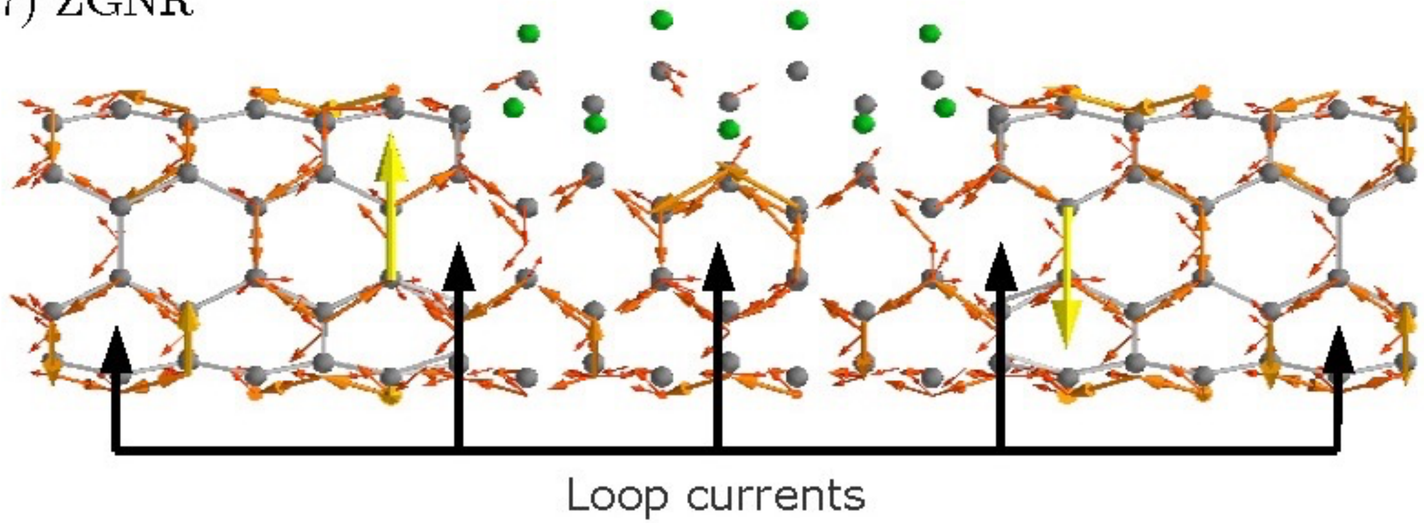
S. Kim and N. Marzari, Phys. Rev. B (2013)

Inelastic quantum transport

(N=5) ZGNR

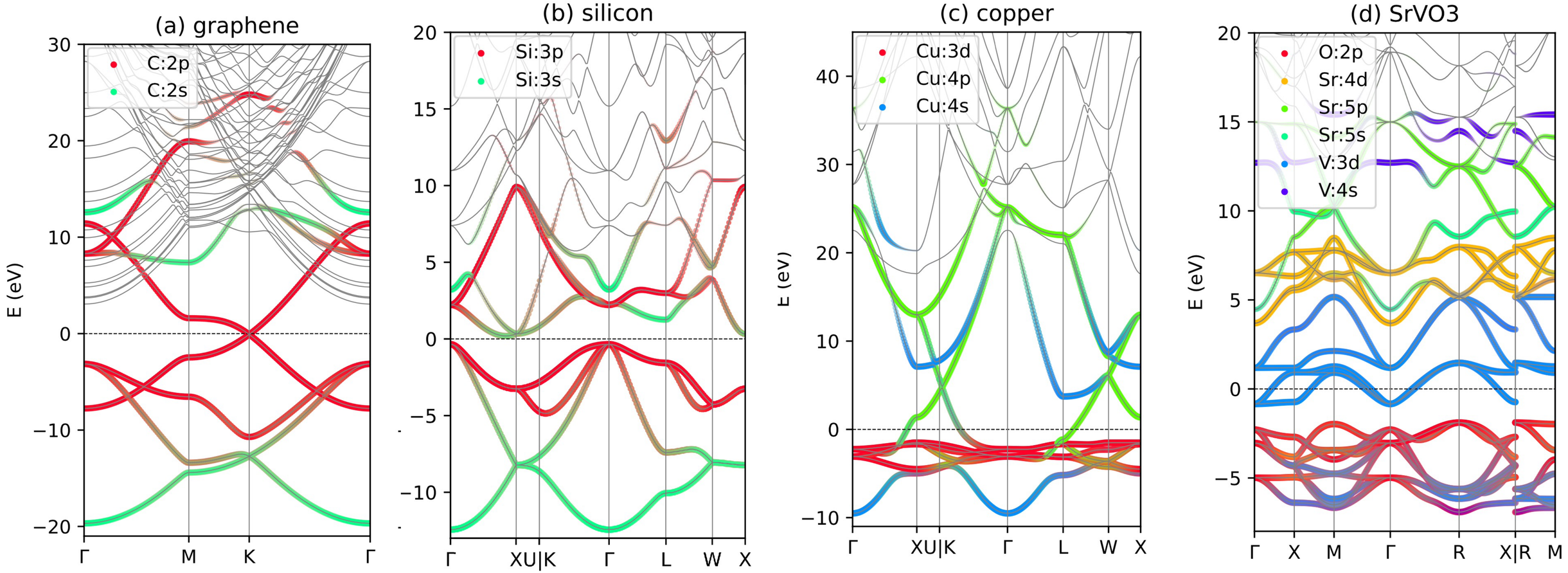


(N=7) ZGNR



2) AUTOMATED WANNIERIZATION

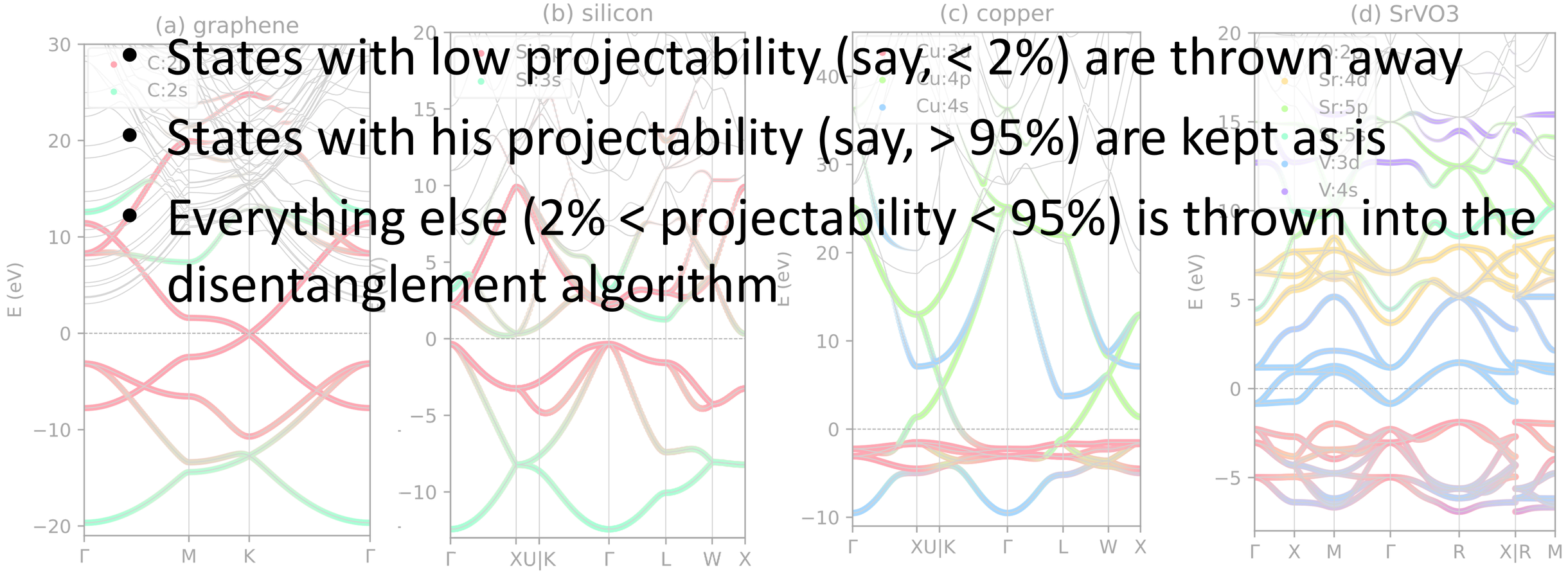
PROJECTABILITY DISENTANGLEMENT



J. Qiao, G. Pizzi, and N. Marzari, npj Computational Materials 9, 208 (2023)

PROJECTABILITY DISENTANGLEMENT

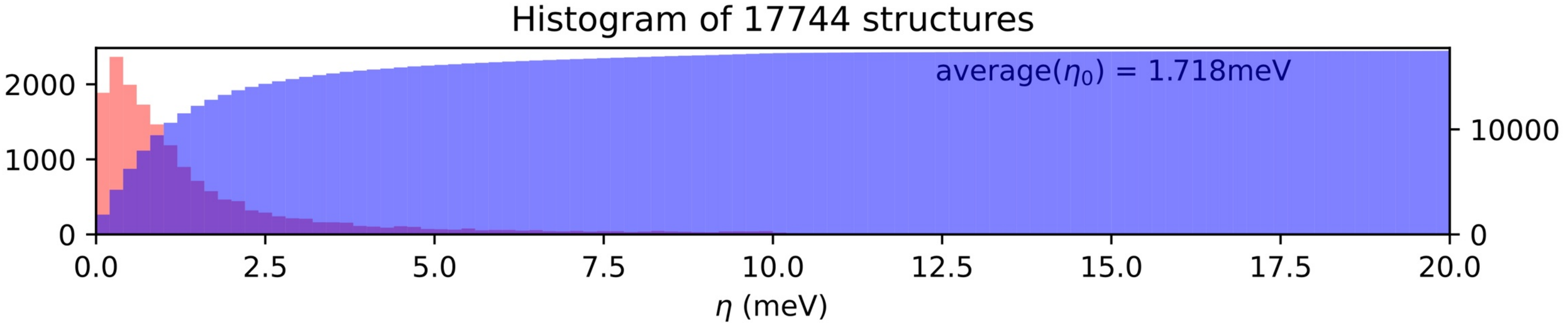
- States with low projectability (say, < 2%) are thrown away
- States with his projectability (say, > 95%) are kept as is
- Everything else (2% < projectability < 95%) is thrown into the disentanglement algorithm



J. Qiao, G. Pizzi, and N. Marzari, npj Computational Materials 9, 208 (2023)

PROJECTABILITY DISENTANGLEMENT

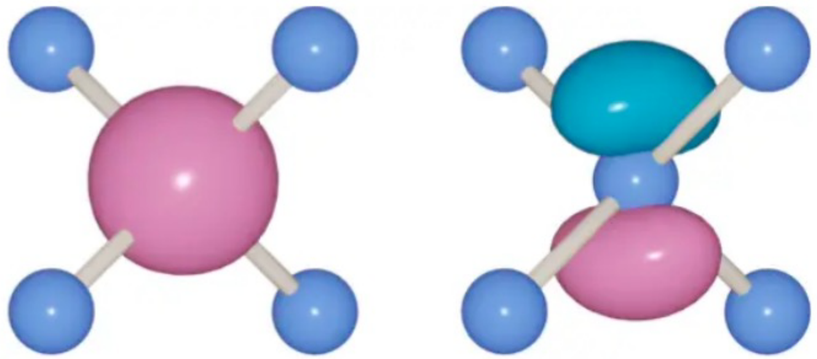
- Automated Wannierization of 17,744 materials, **1,155,049 MLWFs**
- **Average error of 1.7 meV in the band distance η between original and Wannier-interpolated bands**



J. Qiao, G. Pizzi, and N. Marzari, npj Computational Materials 9, 208 (2023)

MANIFOLD REMIXING

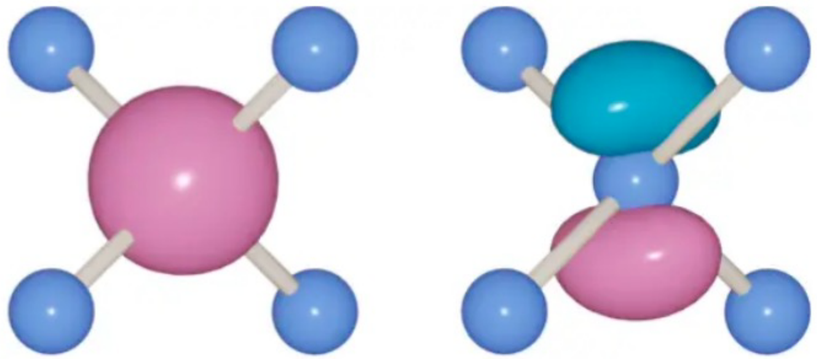
Projectability disentangled: *s* and *p* Wannier functions describing 8 bands (valence bands + conduction)

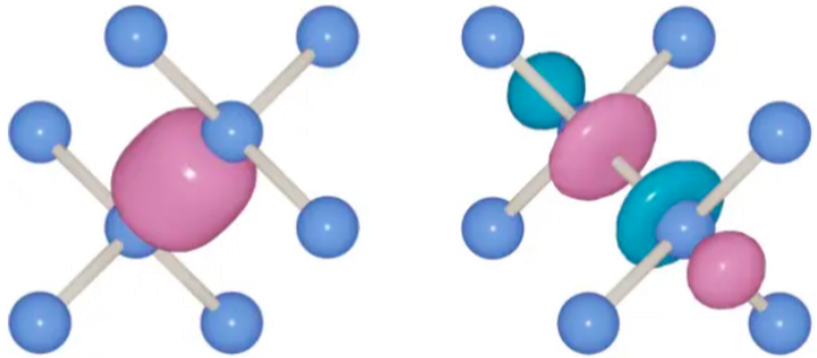


MANIFOLD REMIXING

Projectability disentangled: *s* and *p* Wannier functions describing 8 bands (valence bands + conduction)

These 8 Wannier functions are manifold remixed into 4 “bonding” ones describing only valence bands, and 4 “anti-bonding” describing only the conduction





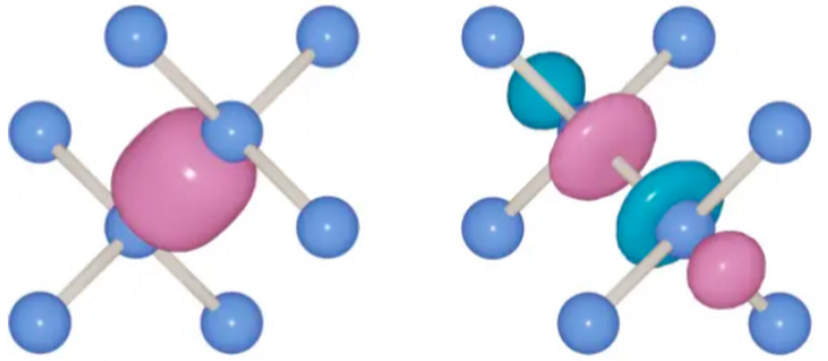
J. Qiao, G. Pizzi, and N. Marzari, npj Computational Materials 9, 206 (2023)

MANIFOLD REMIXING

Separate the submanifolds but keep the gauge continuity: Parallel transport + maximal localization. The final gauge matrices are block-diagonal

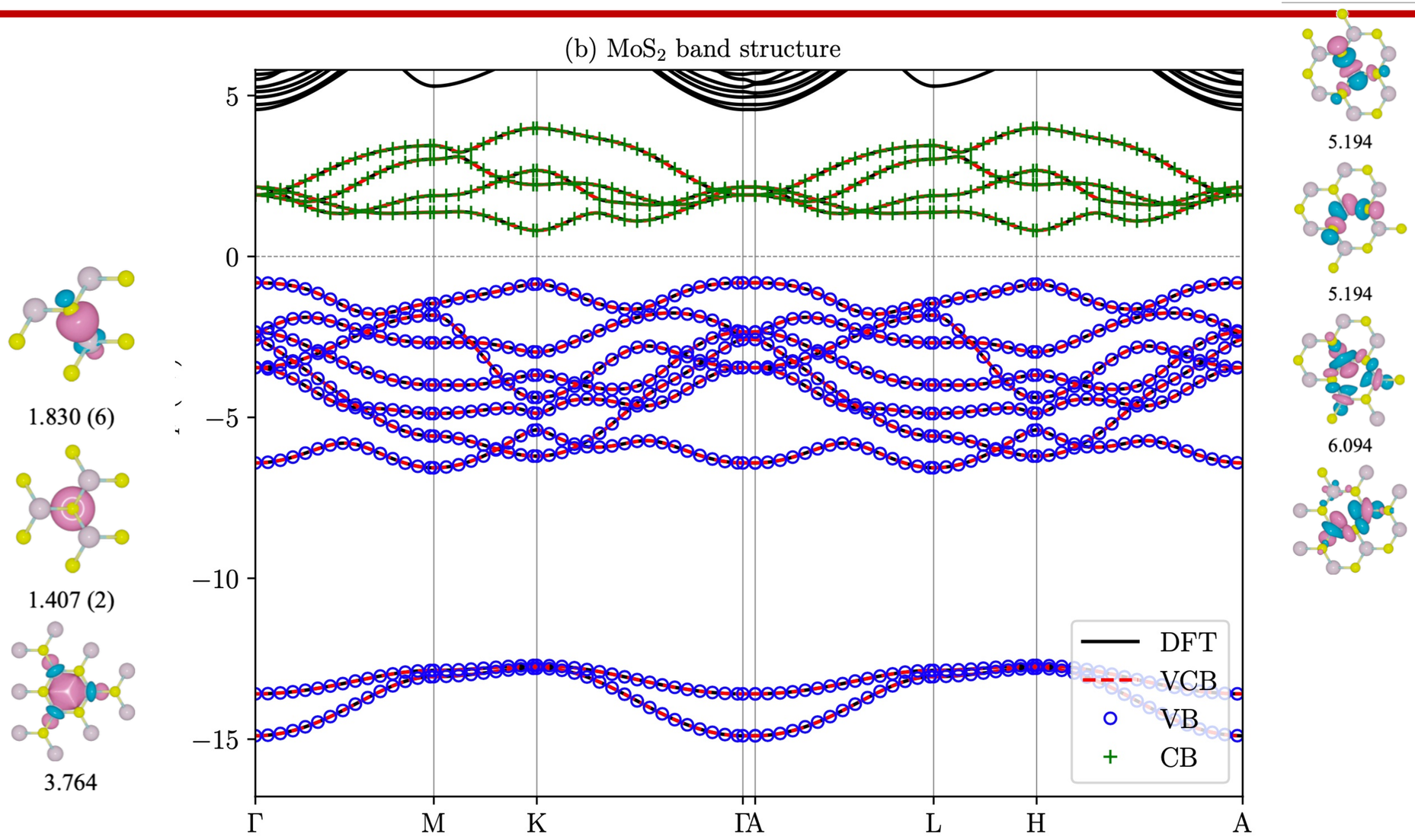
$$\begin{bmatrix} U_{\mathrm{VB}}(\mathbf{k}) & 0 \\ 0 & U_{\mathrm{CB}}(\mathbf{k}) \end{bmatrix}$$

These 8 Wannier functions are manifold remixed into 4 “bonding” ones describing only valence bands, and 4 “anti-bonding” describing only the conduction



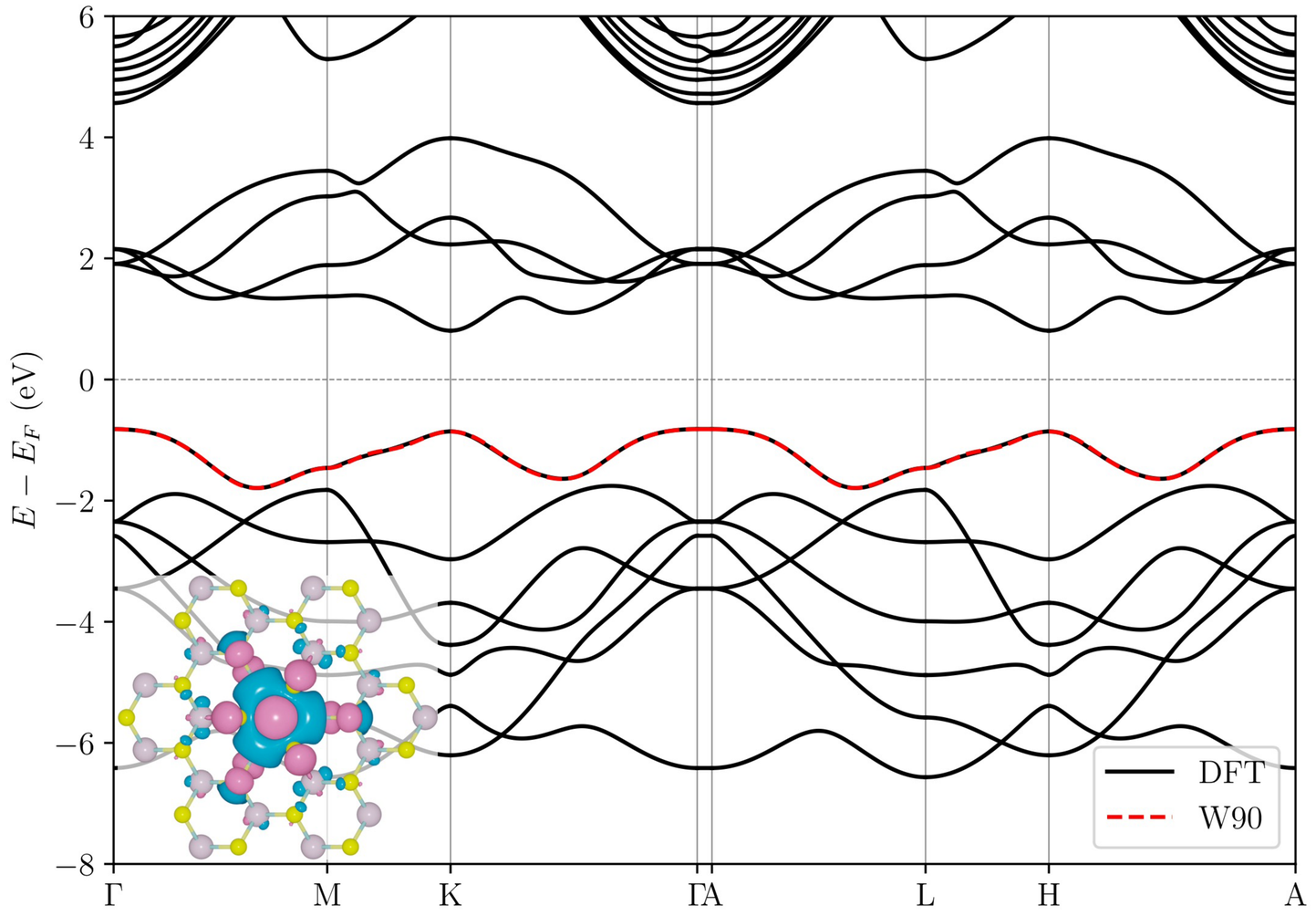
J. Qiao, G. Pizzi, and N. Marzari, npj Computational Materials 9, 206 (2023)

HERE COME M**R**WFs – MANIFOLD REMIXED WFs



J. Qiao, G. Pizzi, and N. Marzari, npj Computational Materials 9, 206 (2023)

HERE COME MRWFs – MANIFOLD REMIXED WFs



J. Qiao, G. Pizzi, and N. Marzari, npj Computational Materials 9, 206 (2023)

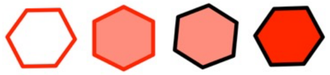
3) KOOPMANS SPECTRAL FUNCTIONALS

For every orbital the expectation value

$$\epsilon_i = \langle \varphi_i | \hat{H}^{\mathrm{DFT}} | \varphi_i \rangle$$

does not depend on the occupation of the orbital

I. Dabo, M. Cococcioni, and N. Marzari, arXiv:0910.2637 (2009)
I. Dabo *et al.*, Physical Review B 82, 115121 (2010)



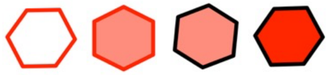
LINEARIZATION

add linear Koopmans

$$E^{\mathrm{KI}} = E^{\mathrm{DFT}} + \sum_i \left[-\int_0^{f_i} \langle \varphi_i | \hat{H}^{\mathrm{DFT}} | \varphi_i \rangle + f_i \qquad \eta_i \right]$$

remove ~quadratic Slater

I. Dabo et al., Physical Review B 82, 115121 (2010)
G. Borghi et al., Physical Review B 90, 075135 (2014)



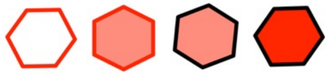
LINEARIZATION

add linear Koopmans

$$E^{\mathrm{KI}} = E^{\mathrm{DFT}} + \sum_i \left[-\int_0^{f_i} \langle \varphi_i | \hat{H}^{\mathrm{DFT}} | \varphi_i \rangle + f_i \int_0^1 \langle \varphi_i | \hat{H}^{\mathrm{DFT}} | \varphi_i \rangle \right]$$

remove ~quadratic Slater

I. Dabo et al., Physical Review B 82, 115121 (2010)
G. Borghi et al., Physical Review B 90, 075135 (2014)



SCREENING

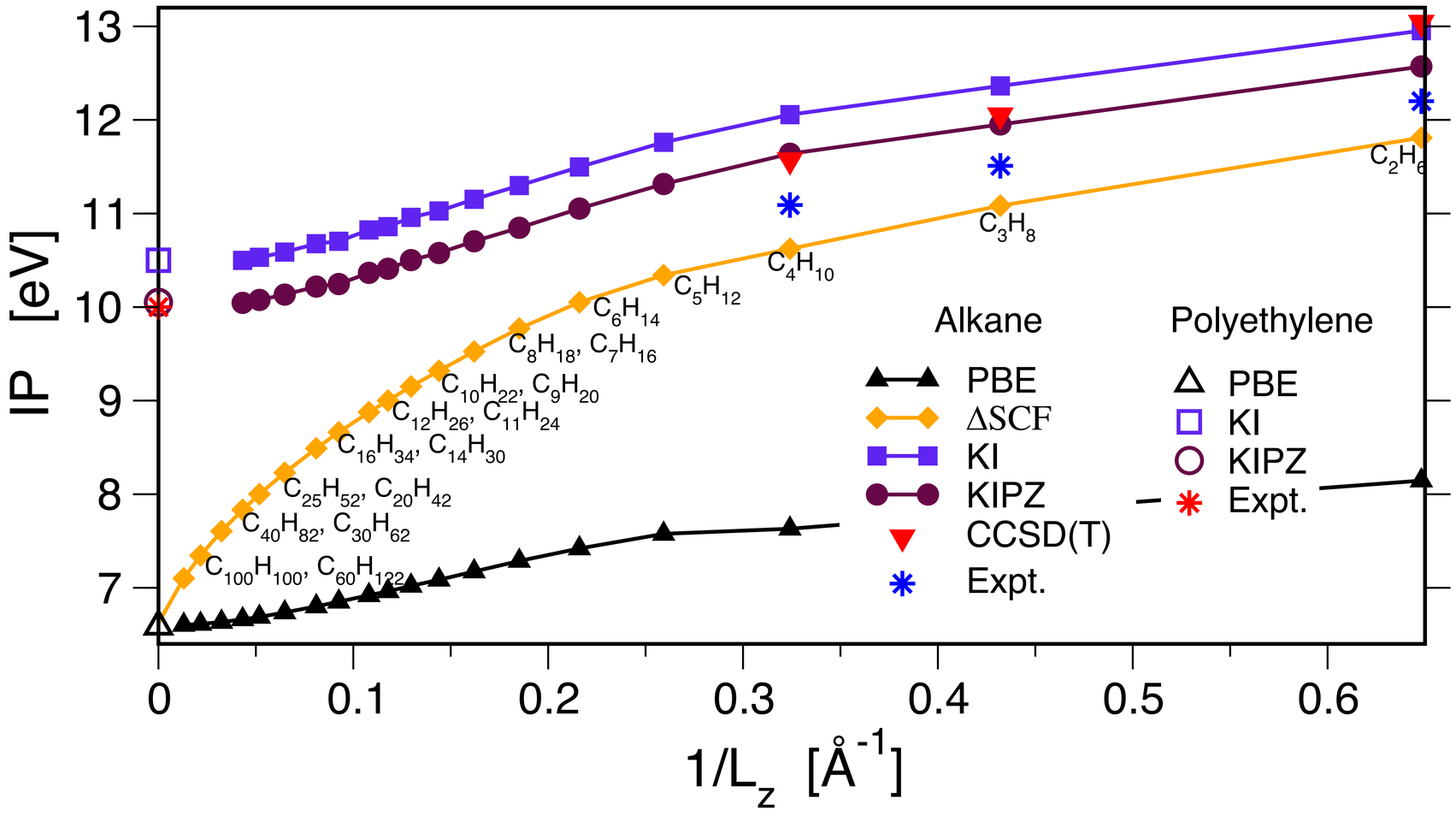
$$E^{\mathrm{KI}} = E^{\mathrm{DFT}} + \sum_i \alpha_i \left[- \int_0^{f_i} \langle \varphi_i | \hat{H}^{\mathrm{DFT}} | \varphi_i \rangle + f_i \int_0^1 \langle \varphi_i | \hat{H}^{\mathrm{DFT}} | \varphi_i \rangle \right]$$

orbital-dependent screening coefficient

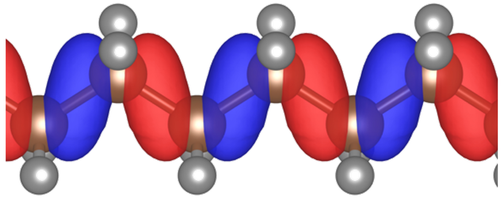
I. Dabo *et al.*, Physical Review B 82, 115121 (2010)

N. Colonna *et al.*, Journal of Chemical Theory and Computation 14, 2549 (2018)

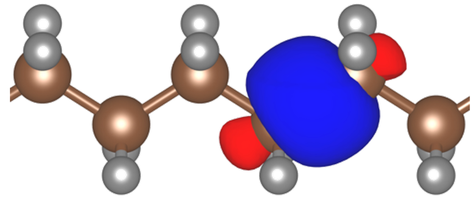
LOCALIZATION



Canonical orbital



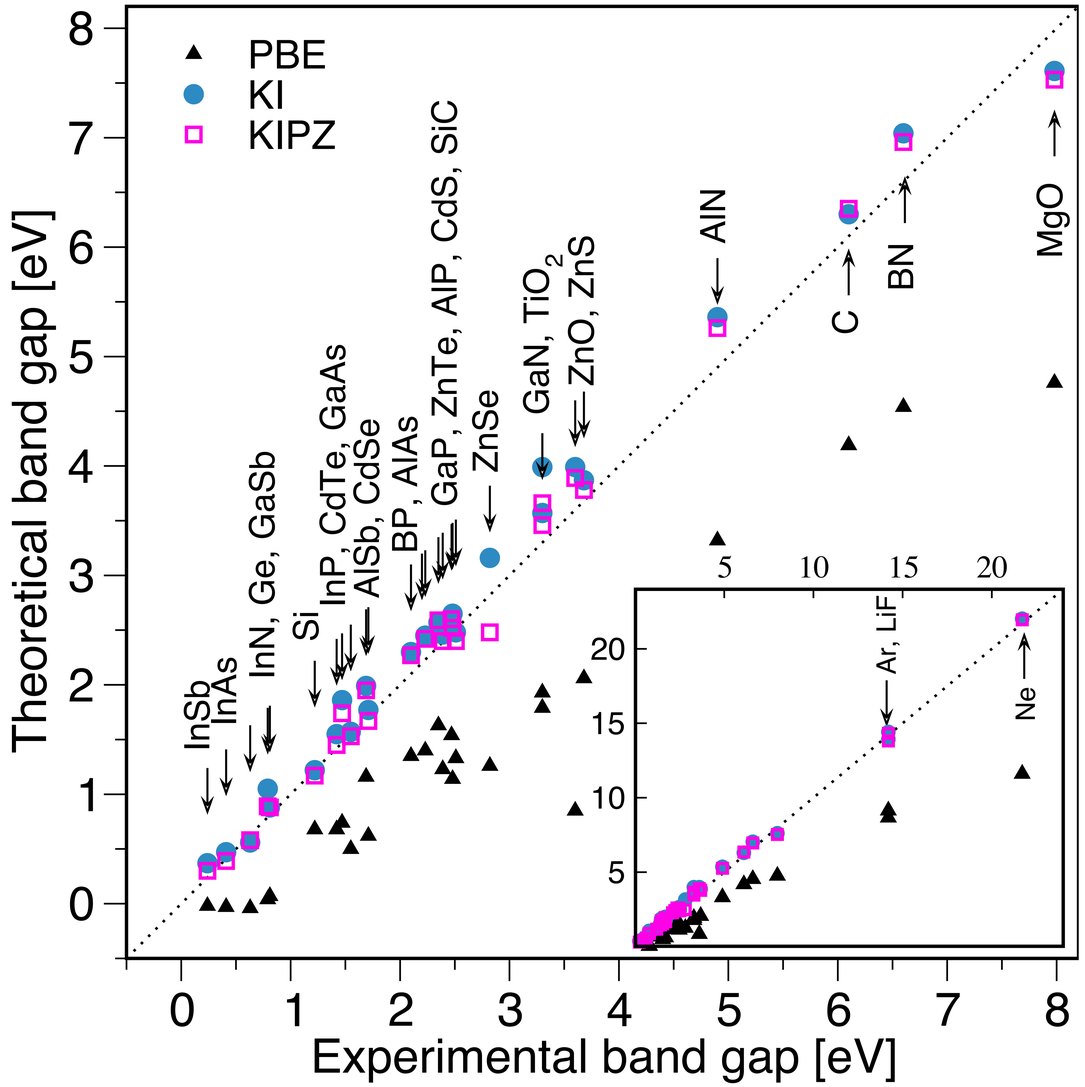
Variational (minimizing) orbital



G. Borghi *et al.*, Physical Review B 91, 155112 (2015)

N.L. Nguyen *et al.*, Physical Review X 8, 02105 (2018)

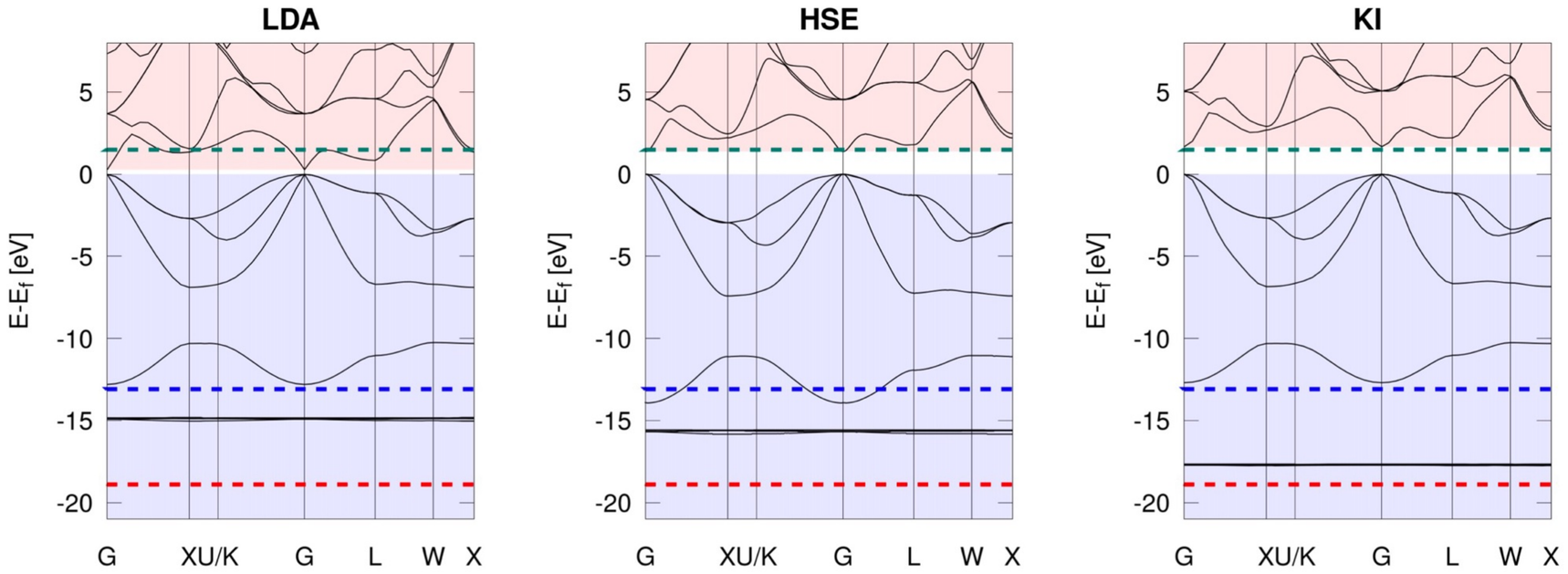
BAND GAPS AND IPs (30 SOLIDS)



MAE (eV)	Gap	IP
PBE	2.54	1.09
G_0W_0	0.56	0.39
QSGW	0.18	0.49
KI	0.27	0.19
KIPZ	0.22	0.21

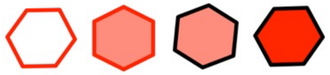
L. Nguyen, N. Colonna, A. Ferretti, and N. Marzari, PRX 8, 021051 (2018)

GALLIUM ARSENIDE

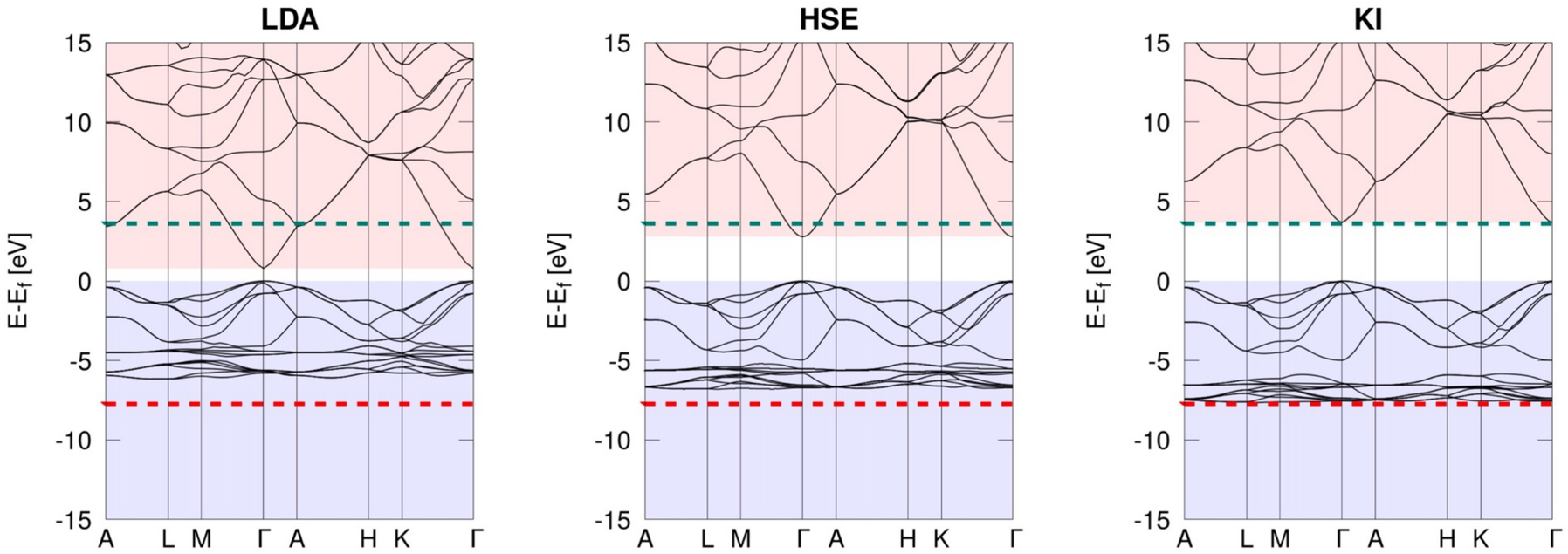


	LDA	HSE	GW_0	$scG\tilde{W}$	KI	Exp.
E_{gap}(eV)	0.19	1.28	1.55	1.62	1.57	1.52
$\langle\varepsilon_d\rangle$(eV)	-14.9	-15.6	-17.3	-17.6	-17.7	-18.9
W(eV)	12.8	13.9	–	–	12.8	13.1

R. De Gennaro, N. Colonna, E. Linscott, and N. Marzari, Phys. Rev. B 106, 035106 (2022)
N. Colonna, R. De Gennaro, E. Linscott, and N. Marzari, JCTC 18, 5435 (2022)
Theoretical values corrected a posteriori for spin-orbit



ZINC OXIDE



	LDA	HSE	GW_0	$scG\tilde{W}$	KI	Exp.
E_{gap}(eV)	0.79	2.79	3.0	3.2	3.62	3.60 (*)
$\langle\varepsilon_d\rangle$(eV)	-5.1	-6.1	-6.4	-6.7	-6.9	-7.5/-8.0

R. De Gennaro, N. Colonna, E. Linscott, and N. Marzari, Phys. Rev. B 106, 035106 (2022)
N. Colonna, R. De Gennaro, E. Linscott, and N. Marzari, JCTC 18, 5435 (2022)
(*) ZPR subtracted from exp value

OPEN-SOURCE CODE: KOOPMANS

Koopmans

a package for performing and automating Koopmans functional calculations

QUANTUMESPRESSO

Contents

https://koopmans-functionals.org/

Edward B. Linscott, Nicola Colonna, Riccardo De Gennaro, Ngoc Linh Nguyen, Giovanni Borghi, Andrea Ferretti, Ismaila Dabo, and Nicola Marzari
koopmans: An Open-Source Package for Accurately and Efficiently Predicting Spectral Properties with Koopmans Functionals,
J. Chem. Theory Comput. 19, 7097–7111 (2023)

REVIEW ARTICLE | INSIGHT
https://doi.org/10.1038/s41563-021-01013-3

nature materials

Check for updates

Electronic-structure methods for materials design

Nicola Marzari[1]✉, Andrea Ferretti[2] and Chris Wolverton[3]

The accuracy and efficiency of electronic-structure methods to understand, predict and design the properties of materials has driven a new paradigm in research. Simulations can greatly accelerate the identification, characterization and optimization of materials, with this acceleration driven by continuous progress in theory, algorithms and hardware, and by adaptation of concepts and tools from computer science. Nevertheless, the capability to identify and characterize materials relies on the predictive accuracy of the underlying physical descriptions, and on the ability to capture the complexity of realistic systems. We provide here an overview of electronic-structure methods, of their application to the prediction of materials properties, and of the different strategies employed towards the broader goals of materials design and discovery.

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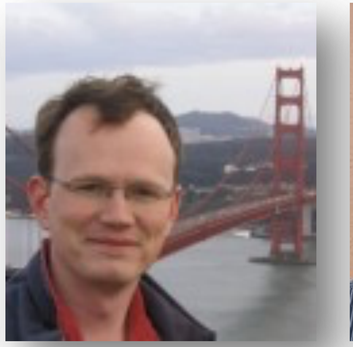
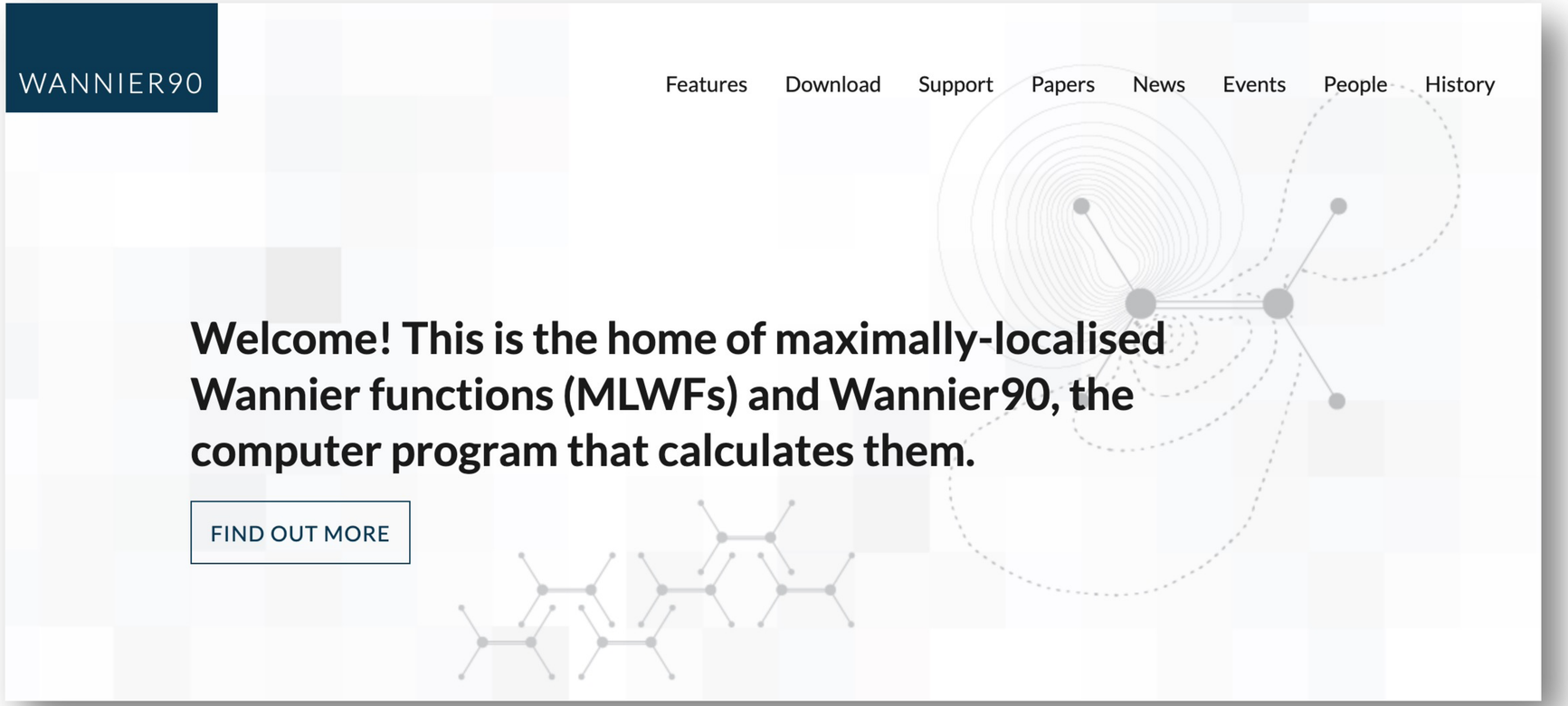



- **Wannier 90:** Arash Mostofi (Imperial College, London), Jonathan Yates (University of Oxford), Giovanni Pizzi (EPFL), Junfeng Qiao (EPFL)
- **Transport:** Young-Su Lee (MIT-), Elise Li (MIT-), Matt Shelley (Imperial), Nicolas Poilvert (MIT), Giovanni Cantele (University of Naples), S. Kim (MIT)
- **Koopmans:** Nicola Colonna (PSI), Andrea Ferretti (CNR), Edward Linscott (PSI), Antimo Marrazzo (SISSA), Riccardo de Gennaro (EPFL), Linh Nguyen (EPFL)




http://www.wannier.org/



Maximally localized Wannier functions: Theory and applications
Nicola Marzari, Arash A. Mostofi, Jonathan R. Yates, Ivo Souza, David Vanderbilt
Rev. Mod. Phys. 84, 1419-1475 (2012)

Wannier90 as a community code: new features and applications
G. Pizzi et al., J. Phys. Cond. Matt. 32, 165902 (2020)


THANKS!