پیوند یا ضدپیوند؟

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سومین مدرسه تابستانه

افق‌های نو در فیزیک

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دانشگاه صنعتی اصفهان

گروه شبیه سازی کوانتومی مواد

Quantum Simulations of Materials
Isfahan University of Technology

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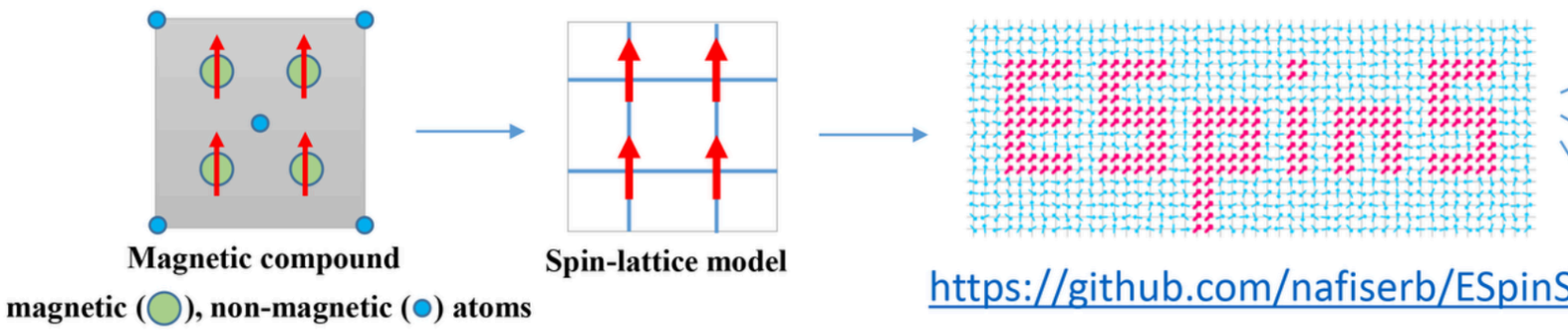
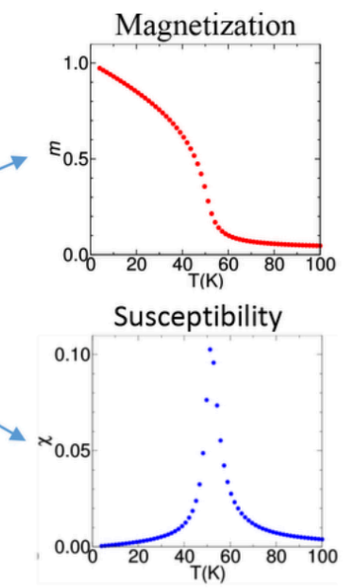
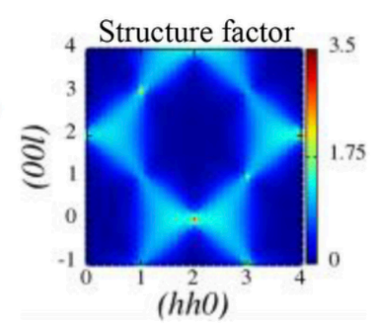
ESpinS: A program for classical Monte-Carlo simulations of spin systems



https://github.com/nafiserb/ESpinS





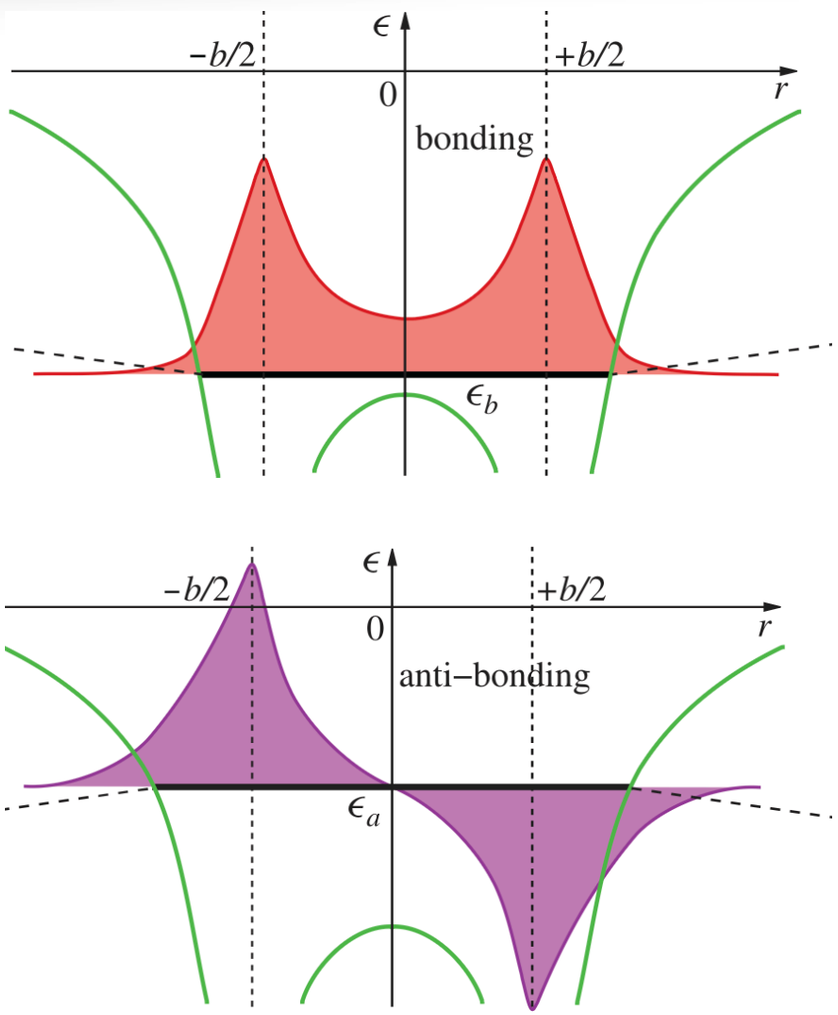
⋮

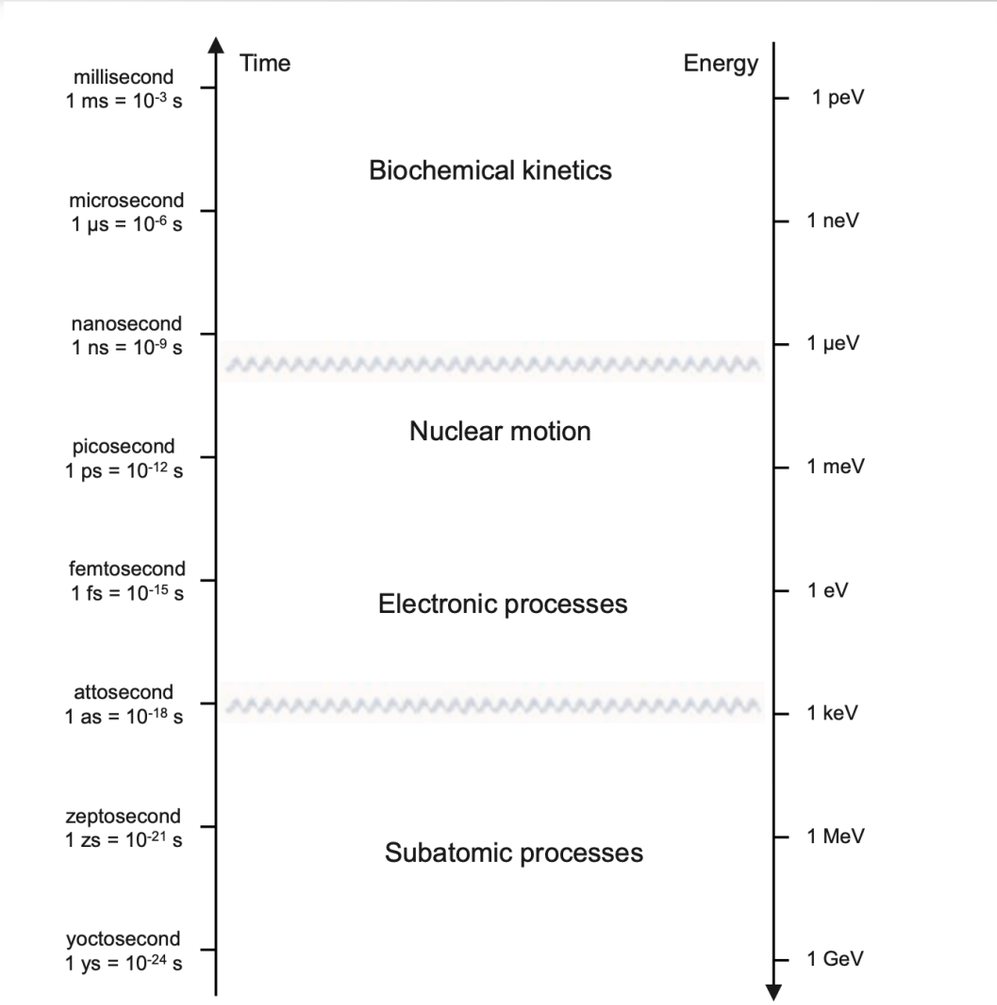
Spin model Hamiltonian:

$$\mathcal{H} = -\frac{1}{2}\sum_{i,j} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j + \frac{1}{2}\sum_{i,j} B_{ij}\left(\mathbf{S}_i\cdot\mathbf{S}_j\right)^2 + \frac{1}{2}\sum_{i,j}\mathbf{D}_{ij}\cdot\left(\mathbf{S}_i\times\mathbf{S}_j\right) + \Delta\sum_i\left(\hat{z}_i\cdot\mathbf{S}_i\right)^2$$

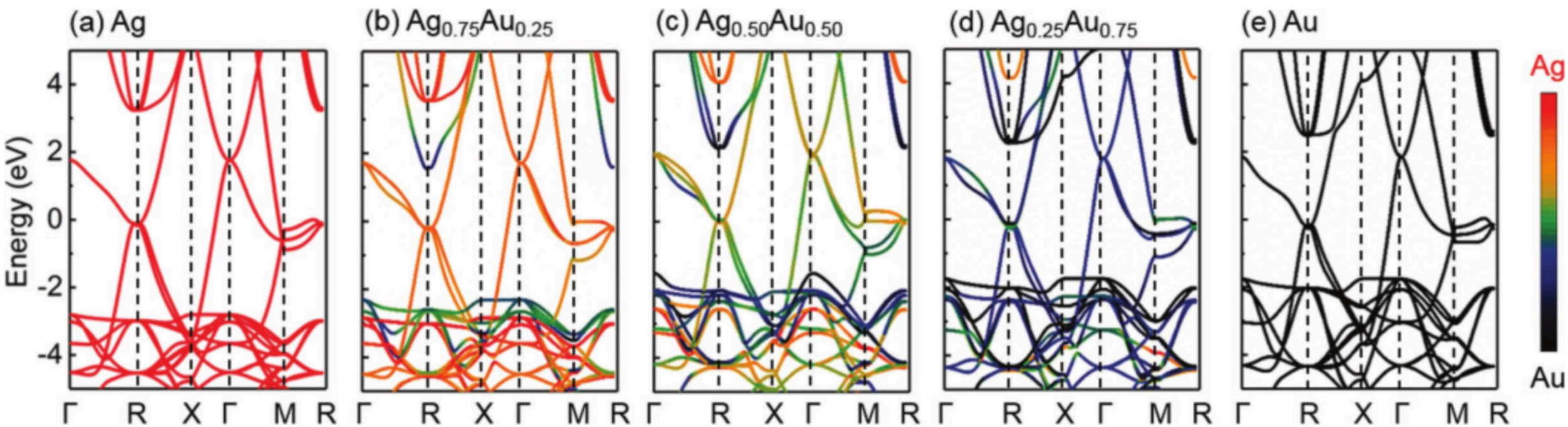
N. Rezaei, M. Alaei and H. Akbarzadeh, Comput. Mater. Sci. 202, 110947 (2022).

پیوند یا ضدپیوند؟



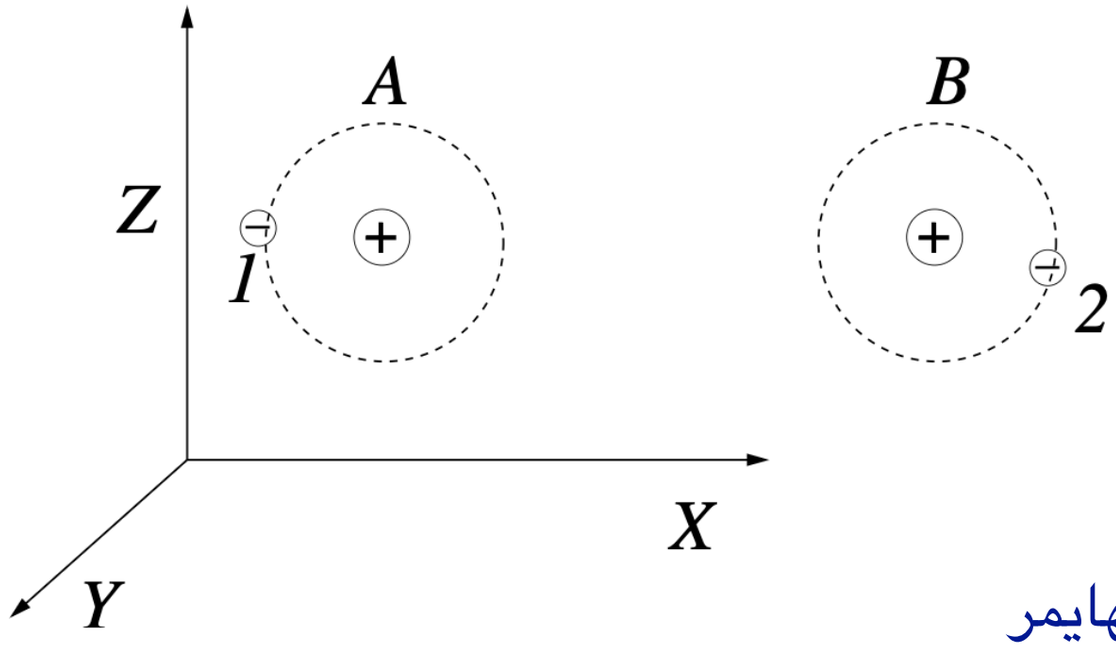


اسپاگتی : ساختار نواری



فهرست مطالب

مولکول هیدروژن



معادله شرودینگر

$$H\psi(\vec{r}_1,\vec{r}_2) = E\psi(\vec{r}_1,\vec{r}_2)$$

هامیلتونی سیستم با در نظر گرفتن تقریب بورن-اپنهایمر

$$H = \left(-\frac{\hbar^2\nabla_1^2}{2m} - \frac{e^2}{|\vec{r}_1-\vec{R}_A|}\right) + \left(-\frac{\hbar^2\nabla_2^2}{2m} - \frac{e^2}{|\vec{r}_2-\vec{R}_B|}\right) - \frac{e^2}{|\vec{r}_1-\vec{R}_B|} - \frac{e^2}{|\vec{r}_2-\vec{R}_A|}$$

$$\langle\vec{r}|\psi\rangle = \psi(\vec{r}) = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-r/a_0}$$

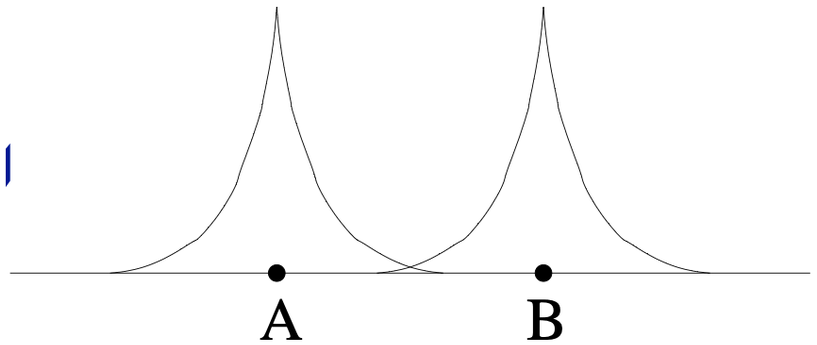
$$H = H_A + H_B - \frac{e^2}{|\vec{r}_1-\vec{R}_B|} - \frac{e^2}{|\vec{r}_2-\vec{R}_A|}$$

$$H_A|1\rangle = \epsilon_{1s}|1\rangle \quad \text{and} \quad H_B|2\rangle = \epsilon_{1s}|2\rangle$$

از کوانتوم بلد هستیم

تراز

اوربیتال



تئوری LCAO

$$|\psi\rangle = \sum_{1}^{2} \psi_i |i\rangle = \psi_1|1\rangle + \psi_2|2\rangle$$

تابع موج بر حسب ترکیب خطی اوربیتال‌های اتمی

انجام کاری معادل Ritz Principle

$$\begin{cases} \langle 1|H(\psi_1|1\rangle + \psi_2|2\rangle) = E\langle 1|(\psi_1|1\rangle + \psi_2|2\rangle) \\ \langle 2|H(\psi_1|1\rangle + \psi_2|2\rangle) = E\langle 2|(\psi_1|1\rangle + \psi_2|2\rangle) \end{cases} \longrightarrow \begin{cases} \langle 1|H|1\rangle\psi_1 + \langle 1|H|2\rangle\psi_2 = E\psi_1 \\ \langle 2|H|1\rangle\psi_1 + \langle 2|H|2\rangle\psi_2 = E\psi_2 \end{cases}$$

$$\begin{cases} \epsilon_0\psi_1 + \gamma\psi_2 = E\psi_1 \\ \gamma\psi_1 + \epsilon_0\psi_2 = E\psi_2 \end{cases} \longrightarrow \begin{pmatrix} \epsilon_0 & \gamma \\ \gamma & \epsilon_0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

$$\det \begin{pmatrix} \epsilon_0 - E & \gamma \\ \gamma & \epsilon_0 - E \end{pmatrix} = 0 \longrightarrow$$

$$(\epsilon_0 - E)^2 - \gamma^2 = 0$$

$$E_{\text{bond}} = \epsilon_0 + \gamma$$

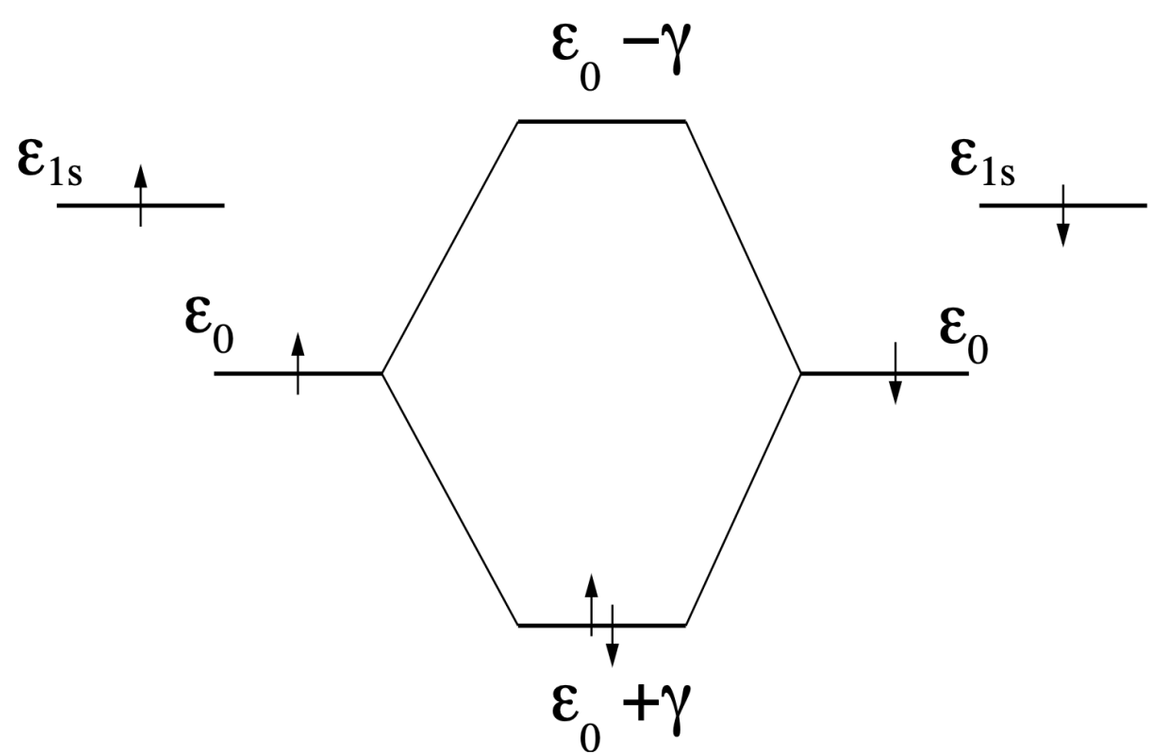
and

$$E_{\text{anti}} = \epsilon_0 - \gamma$$

ترازهای انرژی مولکول هیدروژن

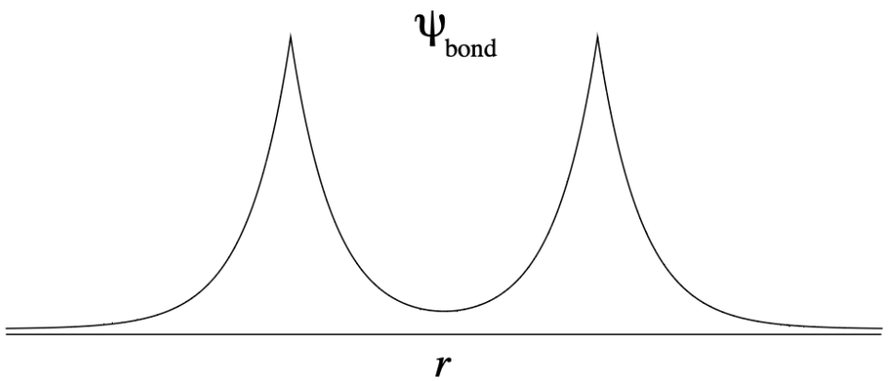
$$E_{\text{bond}} = \epsilon_0 + \gamma \qquad |\psi_{\text{bond}}\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$$

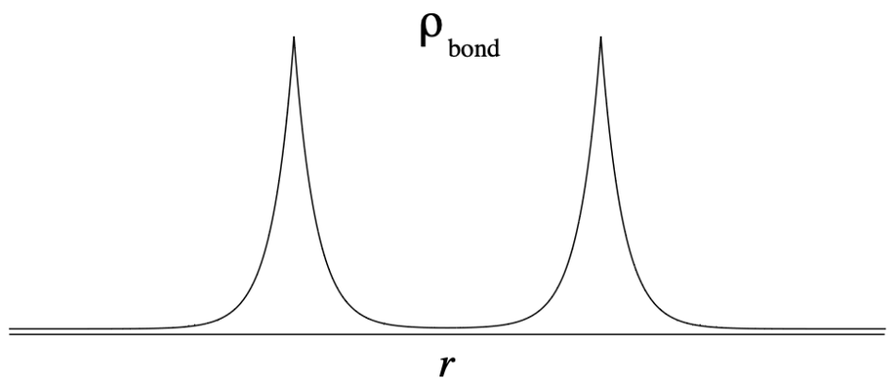
$$E_{\text{anti}} = \epsilon_0 - \gamma \qquad |\psi_{\text{anti}}\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)$$



اوربیتال‌های مولکولی مولکول هیدروژن

Bonding State



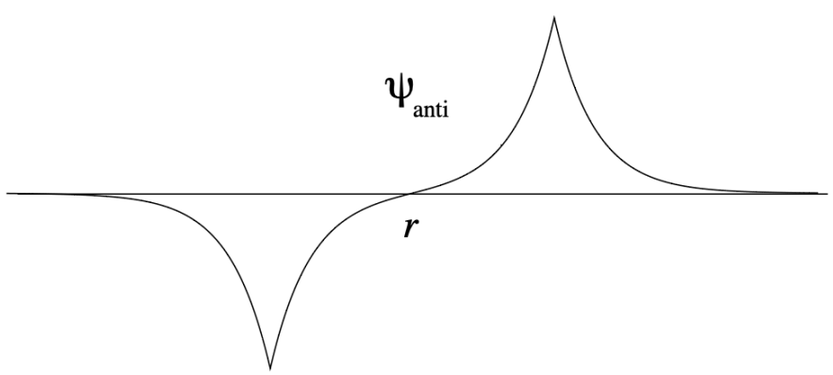


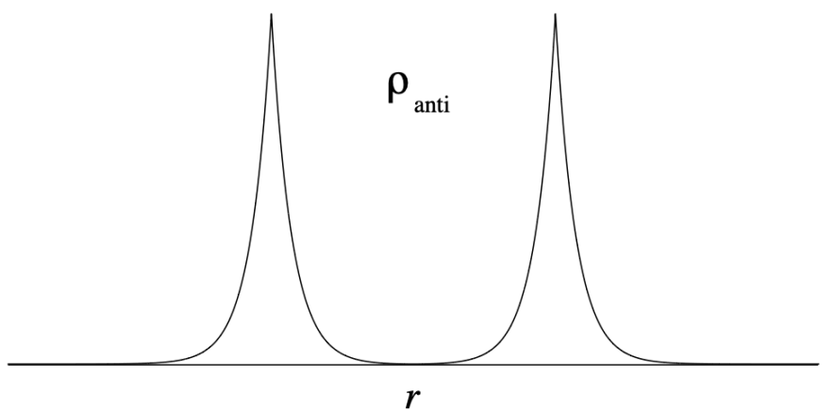
There is charge between the two H atoms → Bond

$$|\psi_{\text{bond}}\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$$

$$|\psi_{\text{anti}}\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)$$

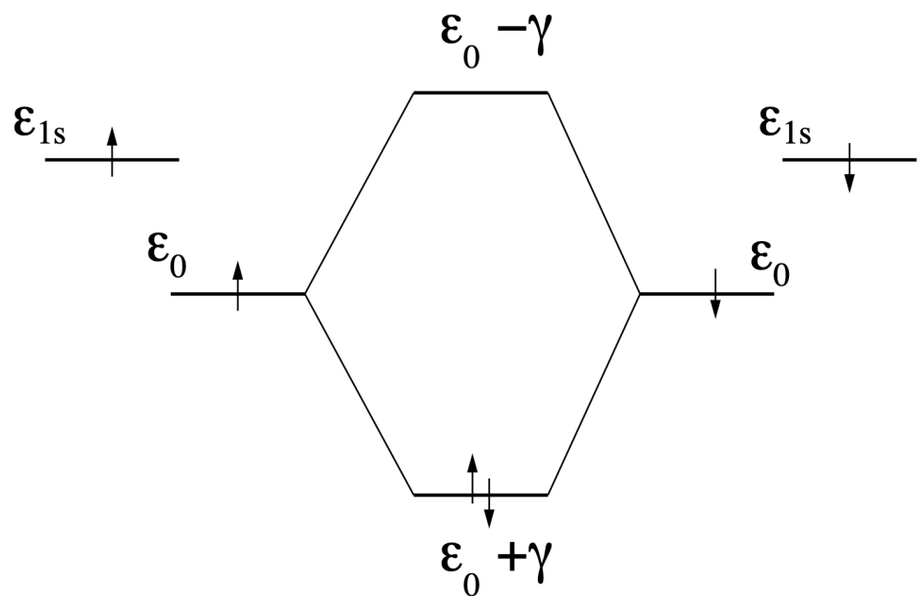
Antibonding State

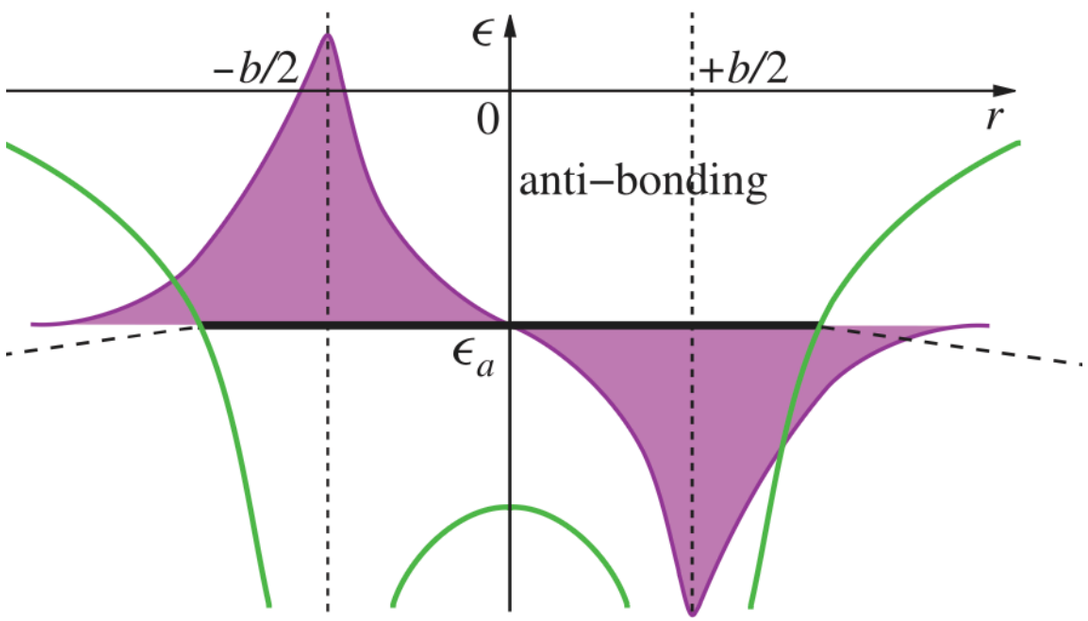


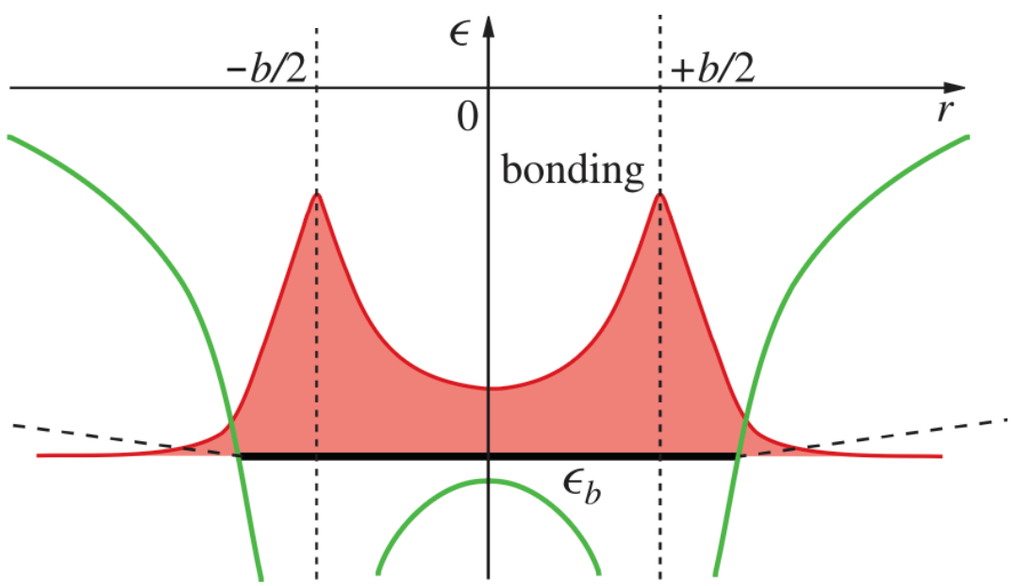


No charge between the two atoms → No bond

نتیجه: حالت پیوندی دارای انرژی کمتر







جامدات

$$H = \frac{1}{2M}\sum_{i=1}^{N_\mathrm{n}} \mathbf{P}_i^2 + \frac{1}{2m_0}\sum_{j=1}^{N_\mathrm{e}} \mathbf{p}_j^2 + \frac{Z^2}{2}\sum_{i,j=1,i\neq j}^{N_\mathrm{n}} V_\mathrm{c}(\mathbf{R}_i - \mathbf{R}_j)$$
$$-Z\sum_{i=1}^{N_\mathrm{n}}\sum_{j=1}^{N_\mathrm{e}} V_\mathrm{c}(\mathbf{r}_j - \mathbf{R}_i) + \frac{1}{2}\sum_{i,j=1,i\neq j}^{N_\mathrm{e}} V_\mathrm{c}(\mathbf{r}_i - \mathbf{r}_j)\,.$$

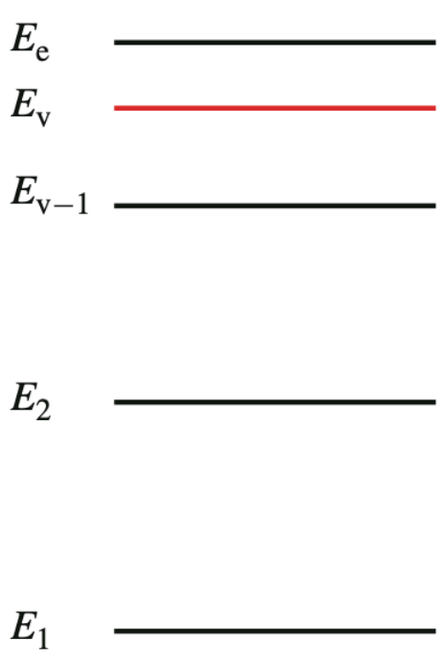
هامیلتونی عمومی جامدات - معادله شرودینگر بس ذره‌ای

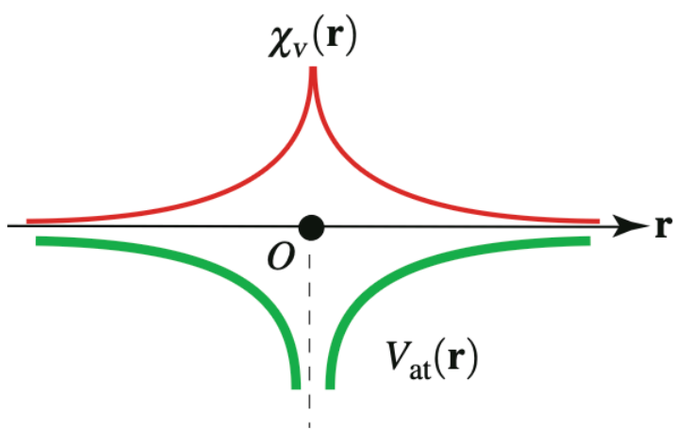
تقریب بورن اپنهایمر
و تقریب مقدار میانگین

تقریب هارتری، هارتری-فوک
و تنگابست- رهیافت DFT

$$\left[\frac{\mathbf{p}^2}{2m_0} + V_\mathrm{at}(\mathbf{r})\right]\chi_n(\mathbf{r}) = E_n\,\chi_n(\mathbf{r})$$

معادله شرودینگر تک ذره‌ای





LCAO

$$\psi_k(\mathbf{r}) = \frac{1}{\sqrt{N_\mathrm{n}}}\sum_{l=1}^{N_\mathrm{n}} a_{k,l}\,\chi_\mathrm{v}(\mathbf{r} - \mathbf{R}_l)$$

$$|\psi_k\rangle = \frac{1}{\sqrt{N_\mathrm{n}}}\sum_{l=1}^{N_\mathrm{n}} a_{k,l}\,|\mathbf{R}_l\rangle$$

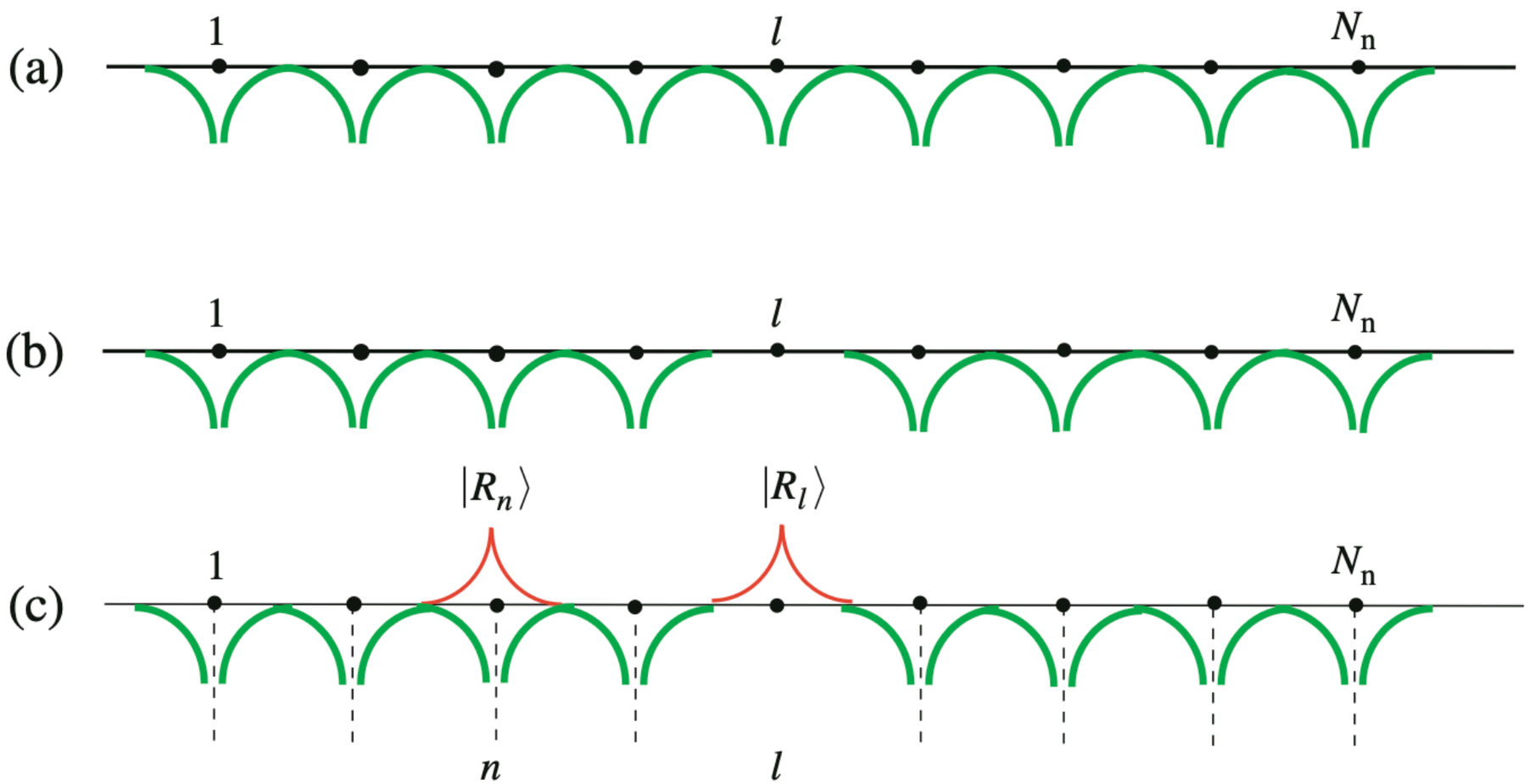
شکل ماتریسی معادله

$$\left[\frac{\mathbf{p}^2}{2m_0} + V_{\mathrm{at}}(\mathbf{r})\right]\chi_n(\mathbf{r}) = E_n\,\chi_n(\mathbf{r})\,.$$

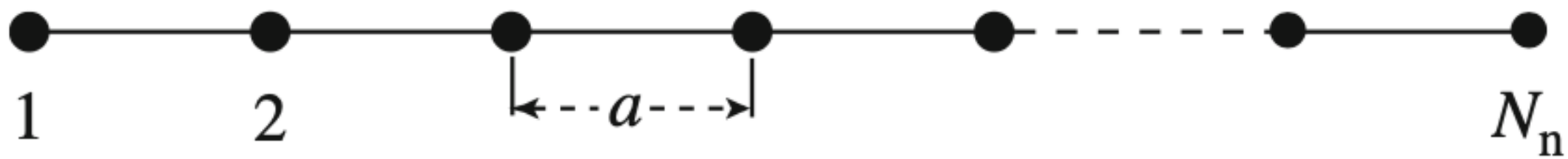
شکل ماتریسی معادله
شرودینگر تک ذره ای
برای زنجیر تک ذره ای

$$-\sum_{l=1}^{N_{\mathrm{n}}} t_{n,l}\,a_{k,l} = (E_k - E_{\mathrm{v}})\,a_{k,n}$$

$$-t_{n,l} = \langle \mathbf{R}_n |\, V_l(\mathbf{r})\, | \mathbf{R}_l \rangle$$



استفاده از تقارن



$$-\sum_{l=1}^{N_n/2-1} t_l(a_{k,n+l}+a_{k,n-l}) = (E_k - E_v + t_0)a_{k,n}$$

$$\psi_k(x) = e^{ikx}u_k(x)\,, \qquad \text{with } u_k(x+a) = u_k(x)$$

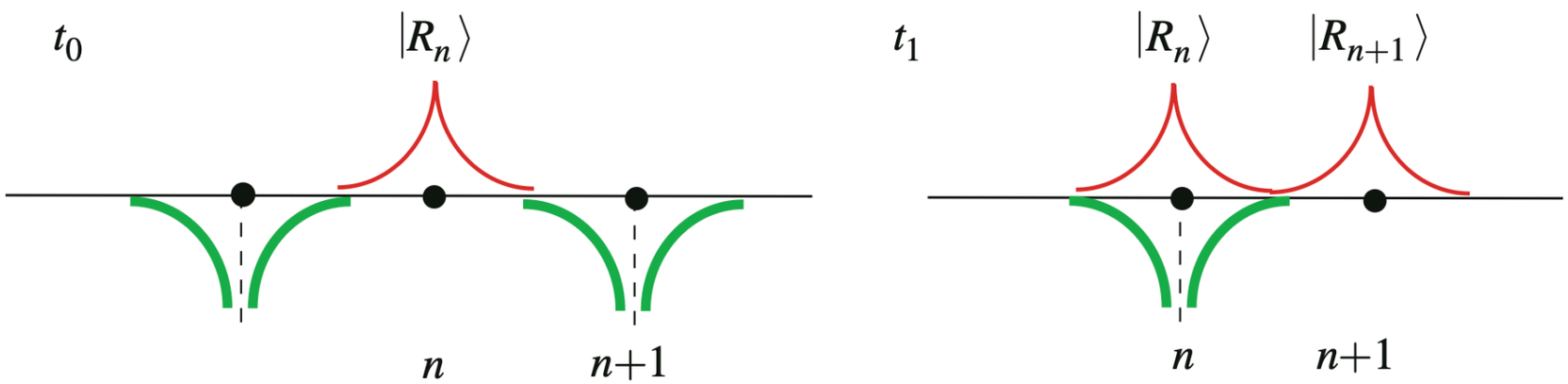
استفاده از توابع بلوخ و شرط مرزی تناوبی

$$\boxed{k = \frac{2\pi m}{N_n a}}\,, \quad m \text{ integer}$$

$$\boxed{a_{k,n} = e^{ikR_n} = e^{ikna}}$$

تقریب نزدیک ترین همسایه

$$t_n = 0 \quad \text{if} \ |n| > 1 \ .$$



$$-t_1(a_{k,n+1} + a_{k,n-1}) = (E_k - E_\mathrm{v} + t_0)a_{k,n} \ .$$

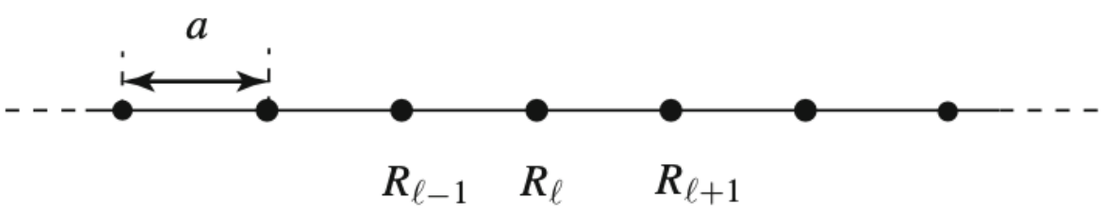
$$\boxed{a_{k,n} = \mathrm{e}^{\mathrm{i}kR_n} = \mathrm{e}^{\mathrm{i}kna}}$$

$$\boxed{E_k = E_\mathrm{v} - t_0 - 2t_1 \cos ka}$$

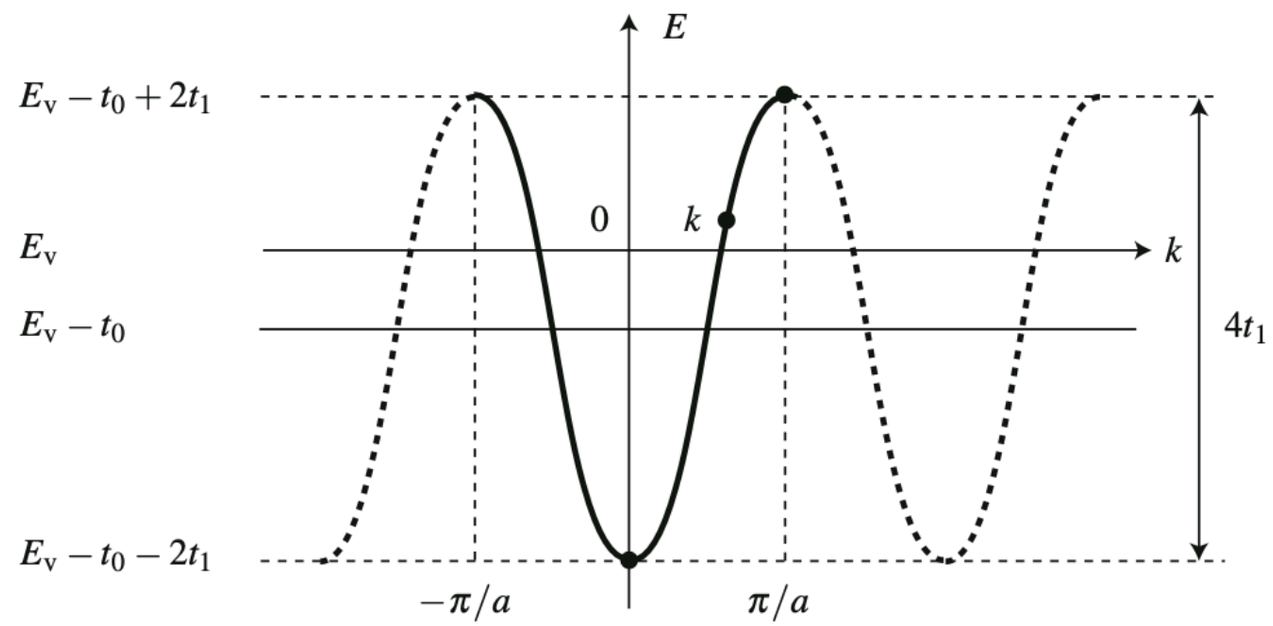
$$\boxed{|\psi_k\rangle = \frac{1}{\sqrt{N_\mathrm{n}}} \sum_{l=1}^{N_\mathrm{n}} \mathrm{e}^{\mathrm{i}kla} |R_l\rangle}$$

ساختار نواری زنجیر اتمی

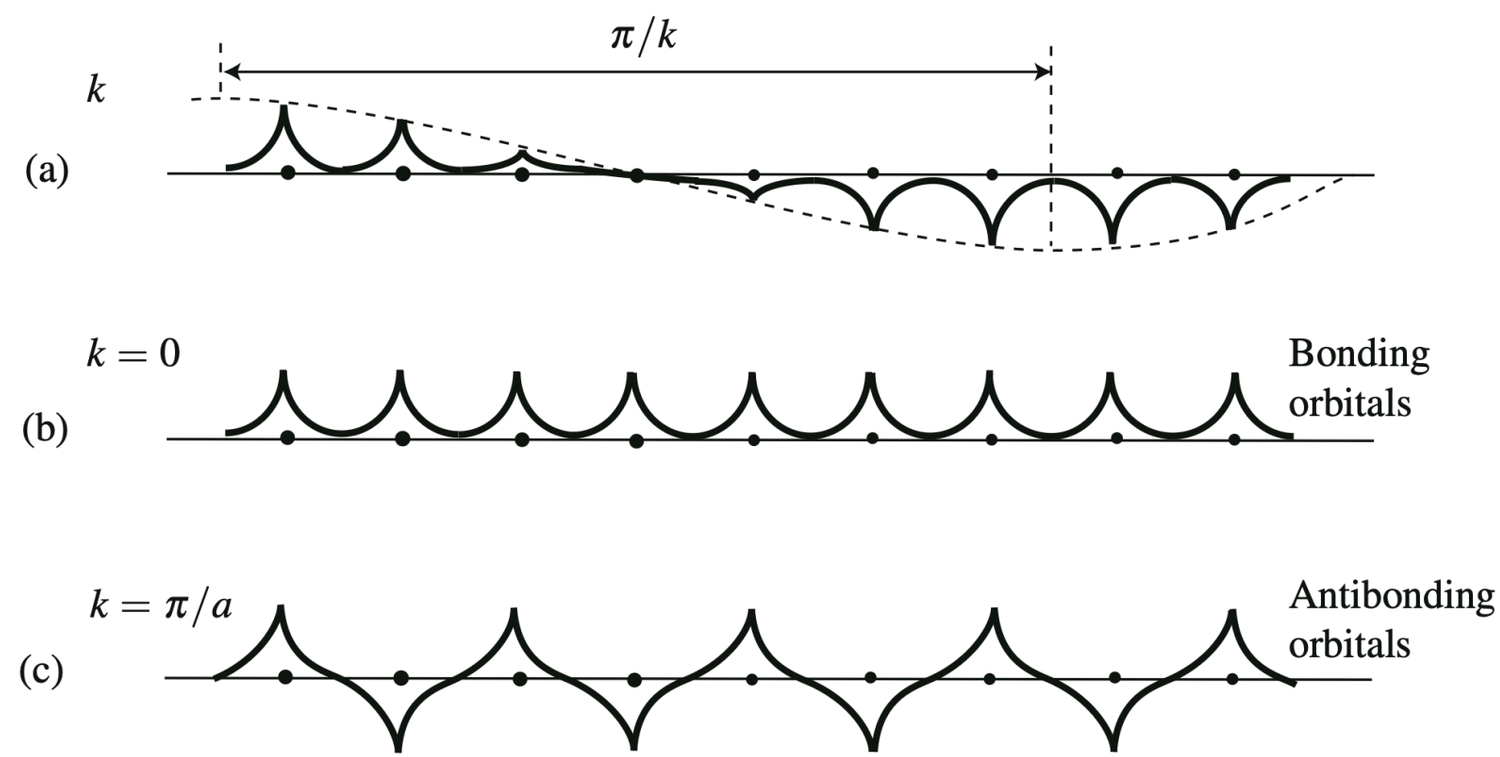
Band Structure



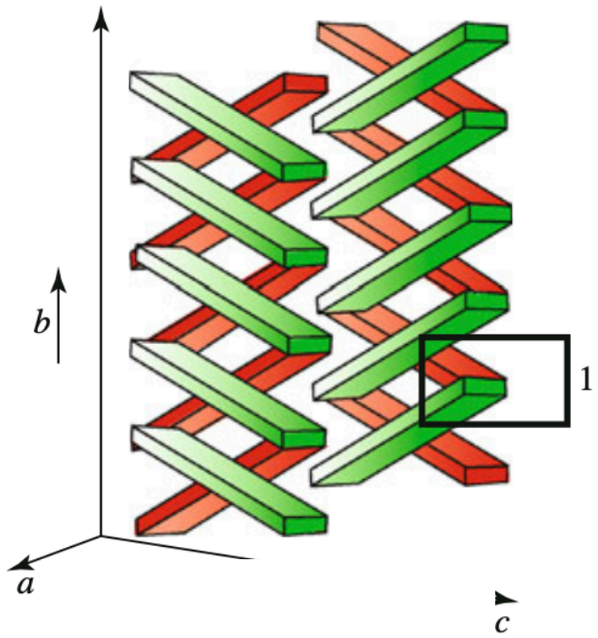
$$E_k = E_\mathrm{v} - t_0 - 2t_1 \cos ka$$

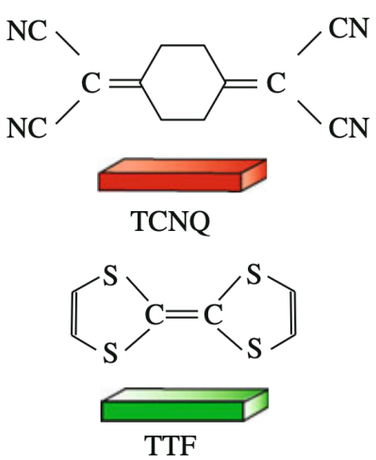


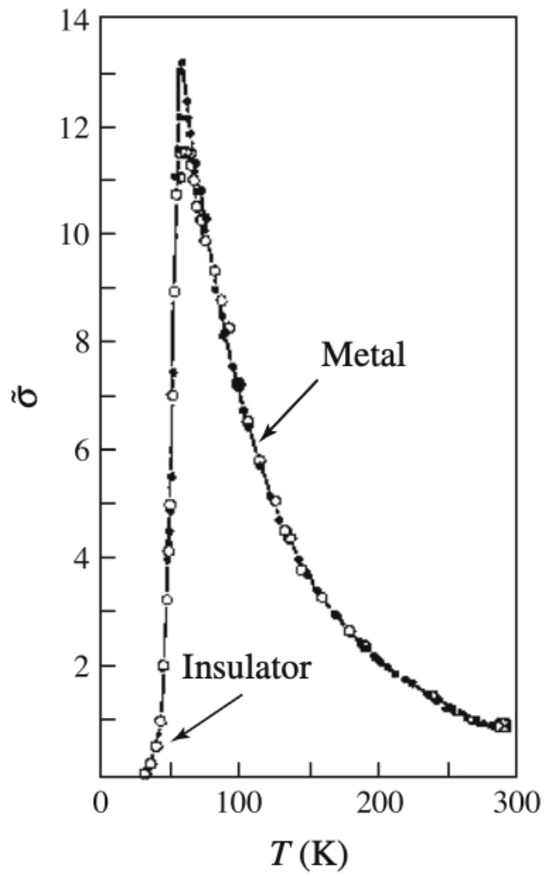
$$|\psi_k\rangle = \frac{1}{\sqrt{N_\mathrm{n}}} \sum_{l=1}^{N_\mathrm{n}} \mathrm{e}^{\mathrm{i}kla} |R_l\rangle$$



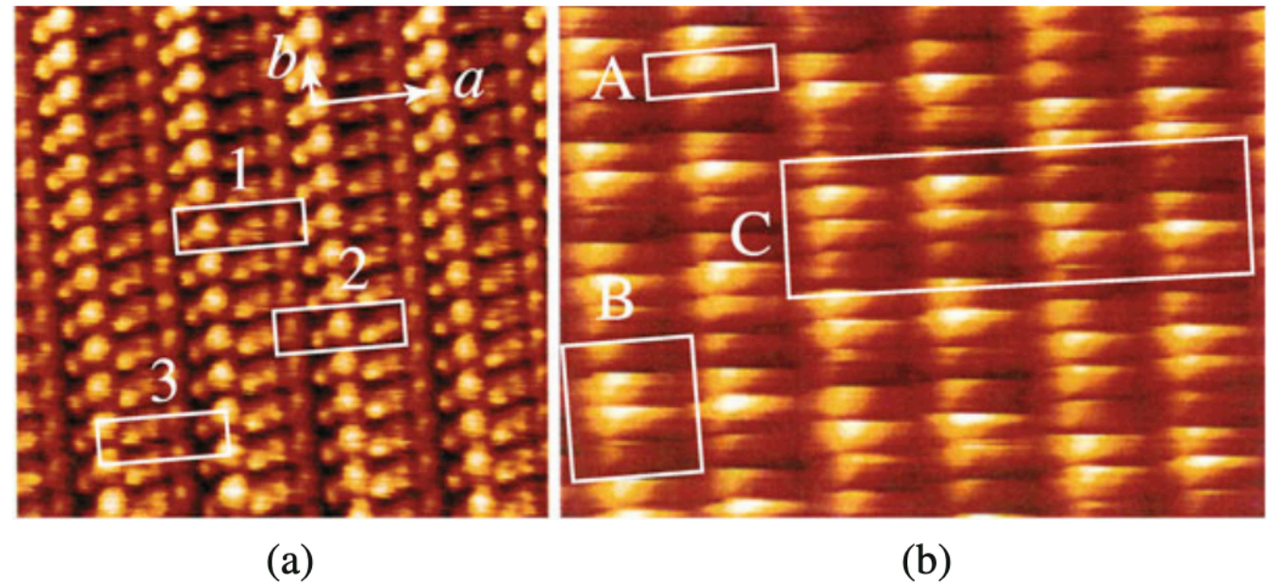
بلور TTF-TCNQ



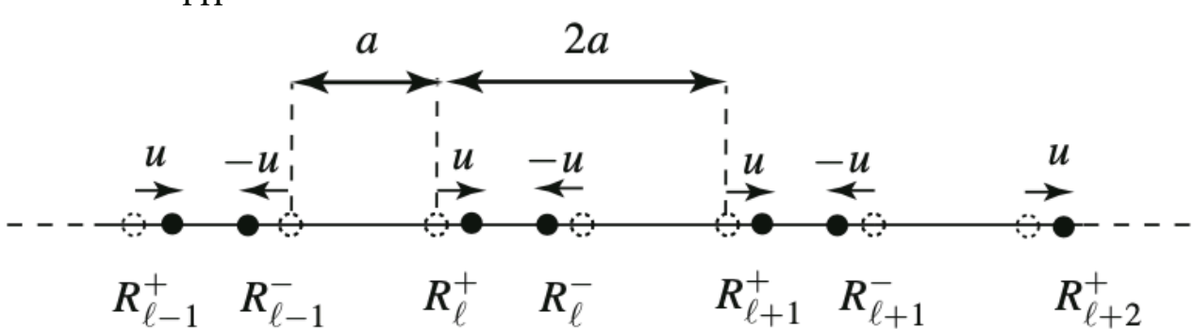




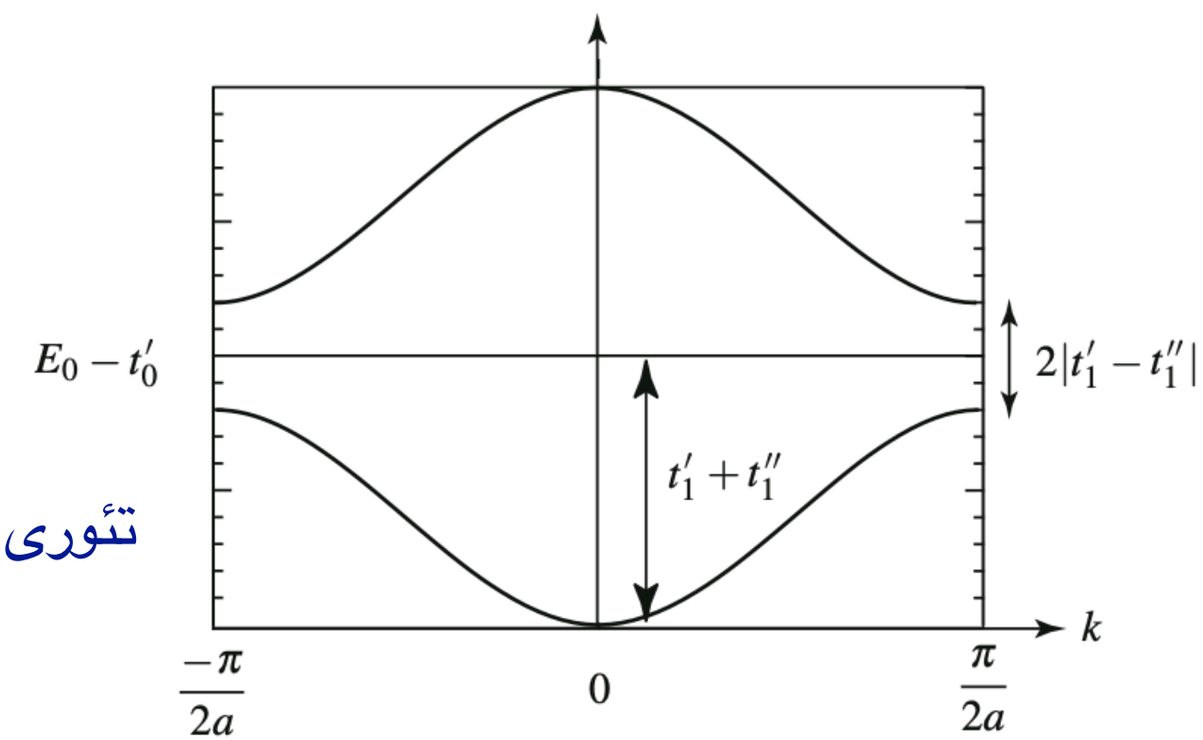
تجربی



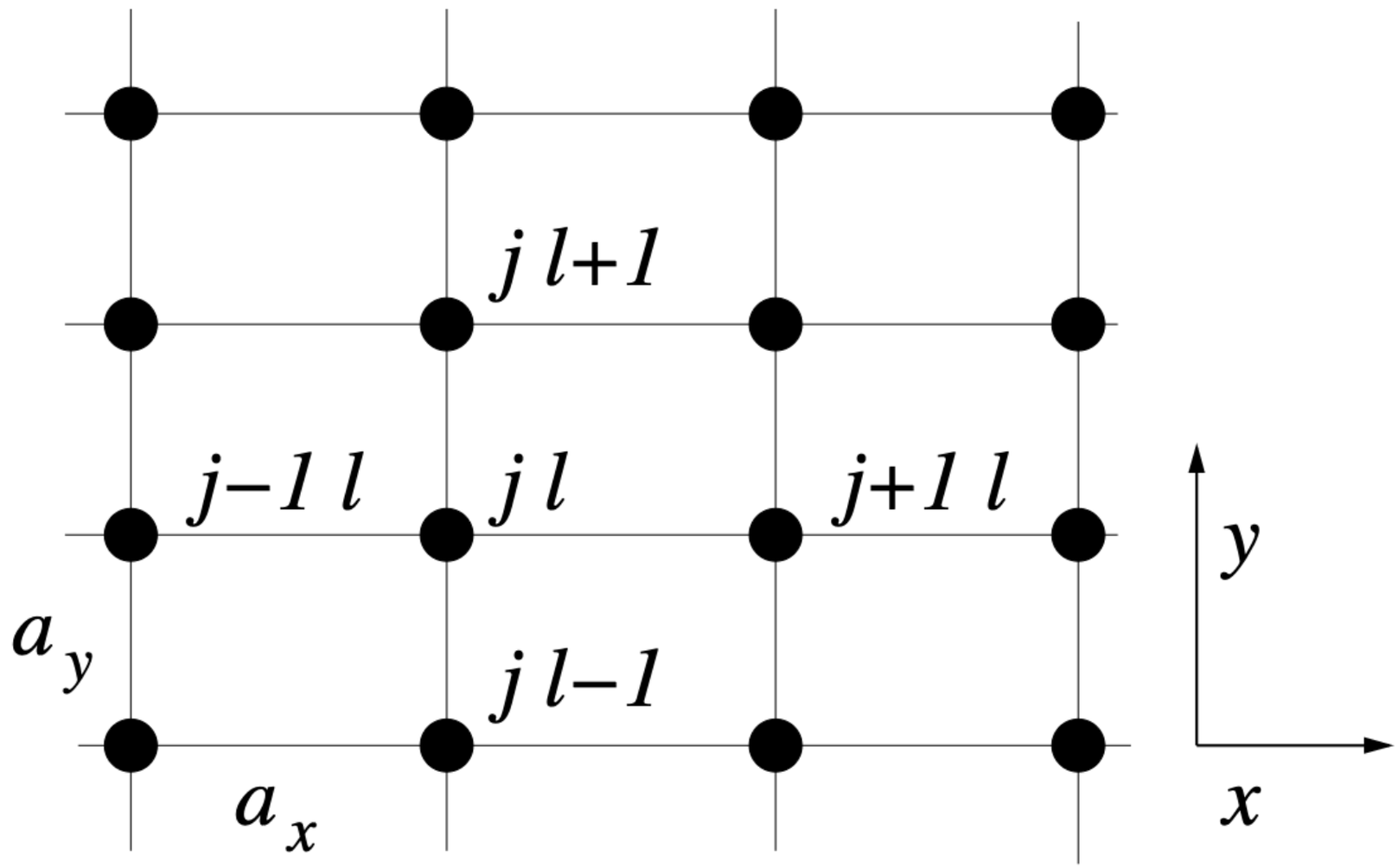
تجربی



تئوری



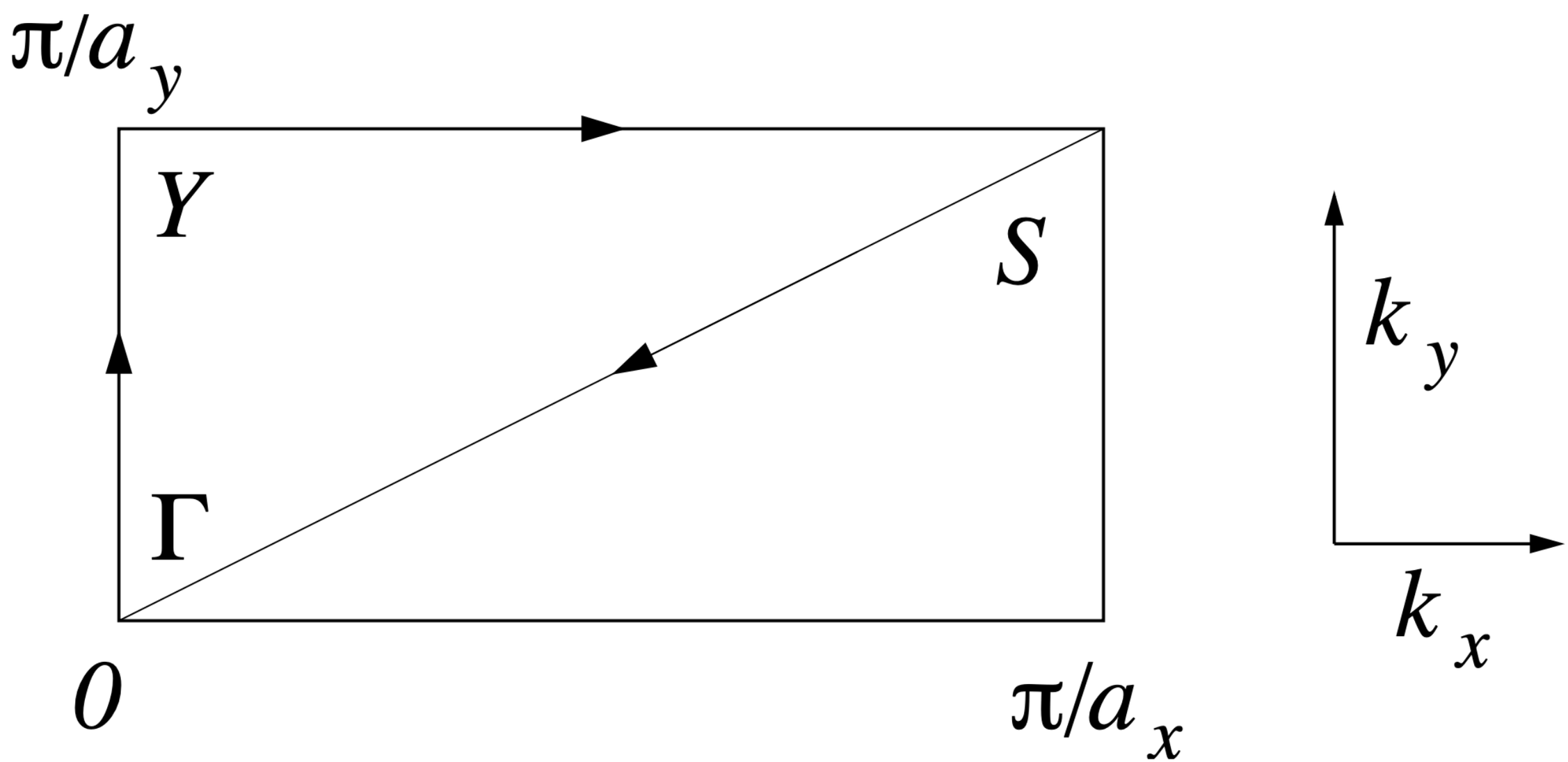
بلور 2D



$$E = \epsilon_0 + 2\gamma_x \cos(k_x a_x) + 2\gamma_y \cos(k_y a_y)$$

نقاط پرتقارن

$$(k_x, k_y) = (0,0) \rightarrow (0, \pi/a_y) \rightarrow (\pi/a_x, \pi/a_y) \rightarrow (0,0)$$

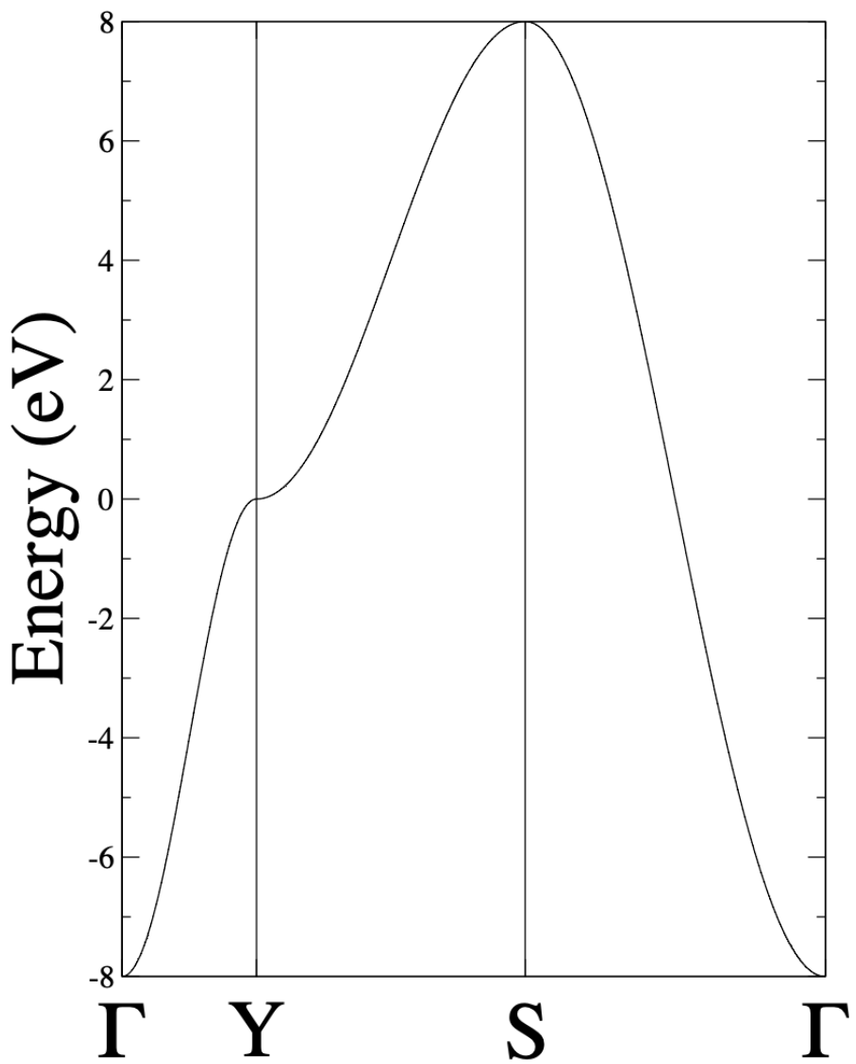


ساختار نواری - مسیر بین نقاط پرتقارن

$$a_y = 2a_x = 2a_0 \qquad E = \epsilon_0 + 2\gamma_x \cos(k_x a_0) + 2\gamma_y \cos(2k_y a_0)$$

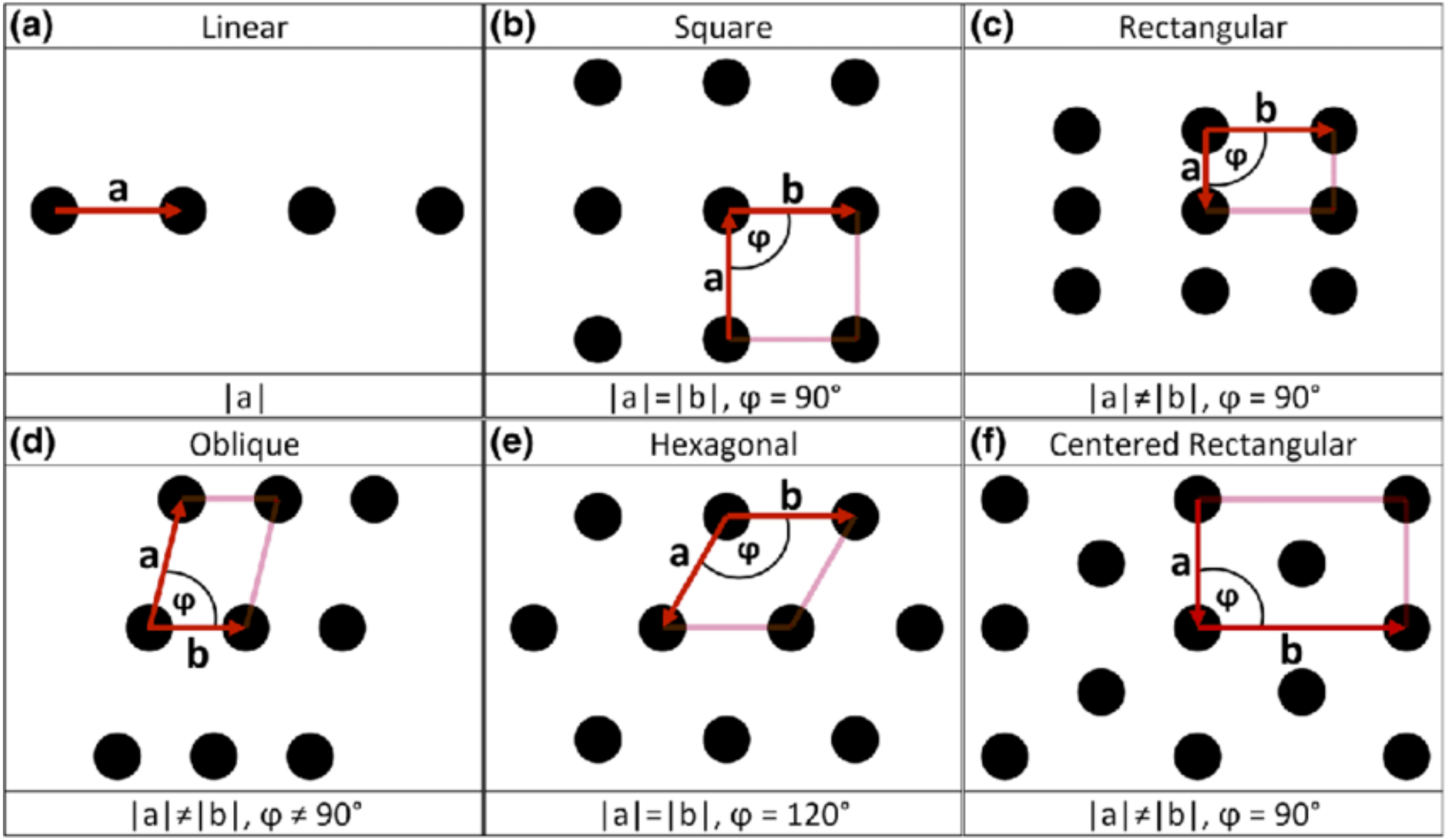
$$(k_x, k_y) = (0,0) \rightarrow (0, \pi/a_y) \rightarrow (\pi/a_x, \pi/a_y) \rightarrow (0,0)$$

$$(k_x, k_y) = \Gamma \rightarrow Y \rightarrow S \rightarrow \Gamma$$



$$\epsilon_0 = 0$$
$$\gamma_x = -2$$
$$\gamma_y = -2$$

ساختارهای 2D



Quasicrystals

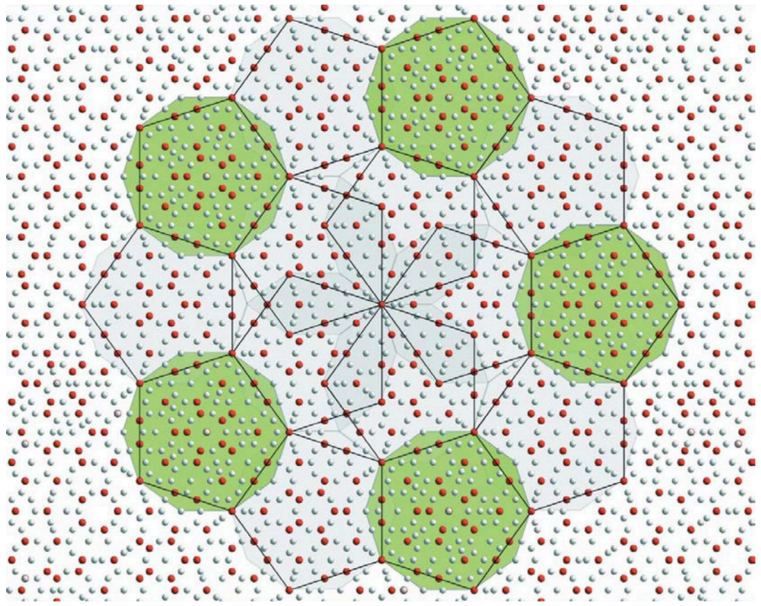
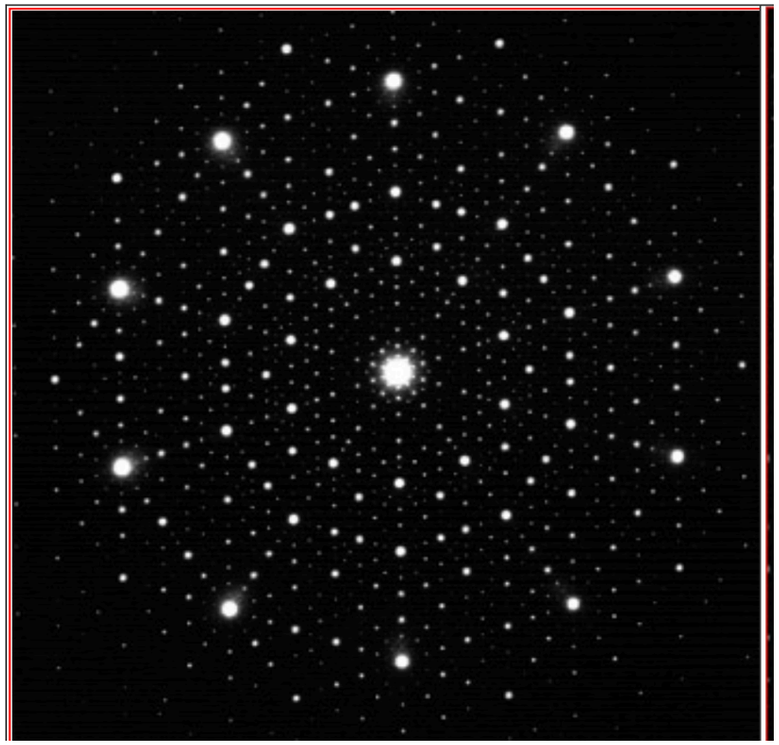
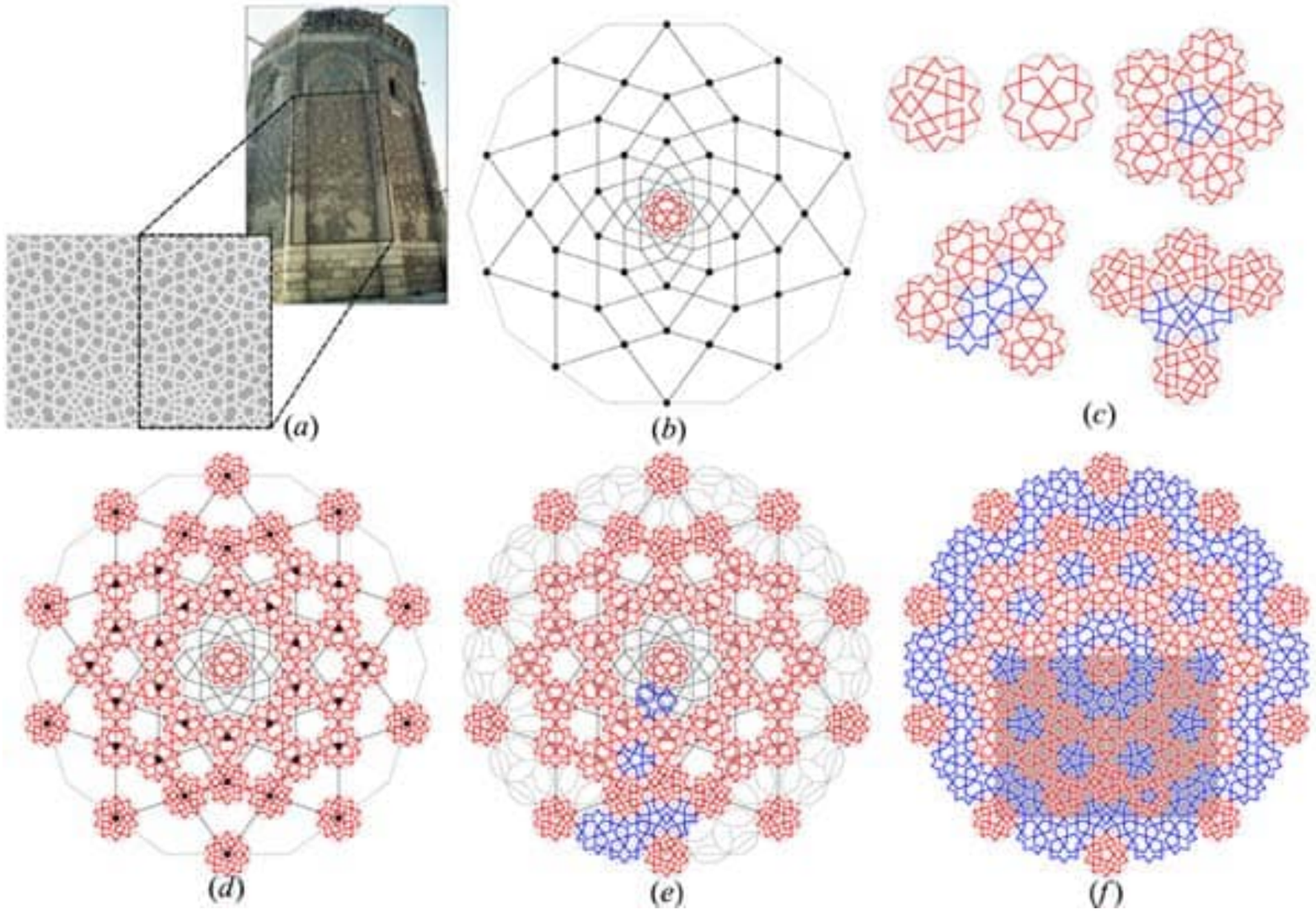


Figure 8. Section perpendicular to the decagonal axis of Al-Co-Ni[36].



The Nobel Prize in Chemistry 2011 is awarded to **Dan Shechtman**



Quasi-periodic pattern at the Gunbad-I Kabud tomb tower in Maragh

گرافین

Electric Field Effect in Atomically Thin Carbon Films

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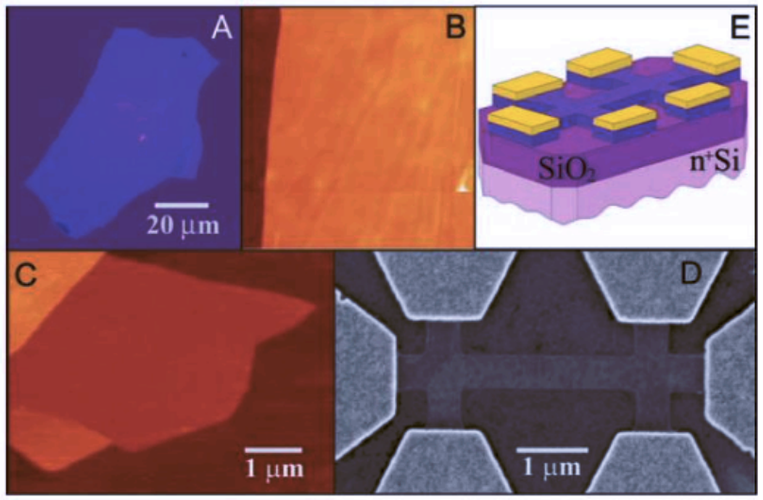
We describe monocrystalline graphitic films, which are a few atoms thick but are nonetheless stable under ambient conditions, metallic, and of remarkably high quality. The films are found to be a two-dimensional semimetal with a tiny overlap between valence and conductance bands, and they exhibit a strong ambipolar electric field effect such that electrons and holes in concentrations up to 10^{13} per square centimeter and with room-temperature mobilities of ~10,000 square centimeters per volt-second can be induced by applying gate voltage.

22 OCTOBER 2004 VOL 306 SCIENCE www.sciencemag.org



Graphene films.

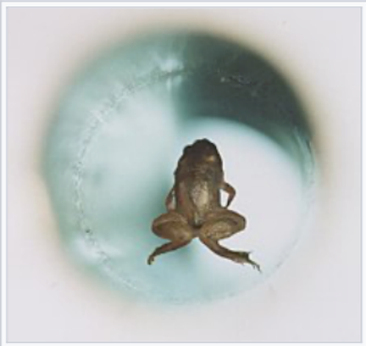
(A) Photograph (in normal white light) of a relatively large multilayer graphene flake with thickness 3 nm on top of an oxidized Si wafer.

(B) Atomic force microscope (AFM) image of 2 μm by 2 μm area of this flake near its edge. Colors: dark brown, SiO_2 surface; orange, 3 nm height above the SiO_2 surface.

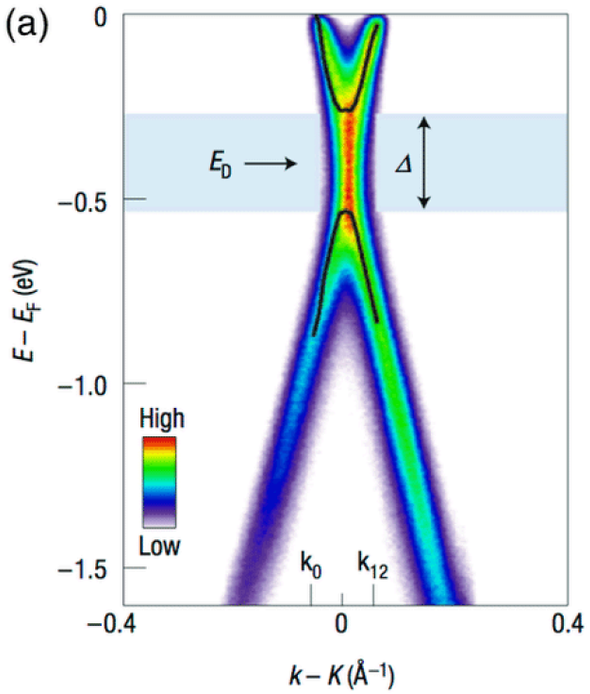
(C) AFM image of single-layer graphene. Colors: dark brown, SiO_2 surface; brown-red (central area), 0.8 nm height; yellow-brown (bottom left), 1.2 nm; orange (top left), 2.5 nm. Notice the folded part of the film near the bottom, which exhibits a differential height of 0.4 nm.

(D) Scanning electron microscope image of one of our experimental devices prepared from FLG.

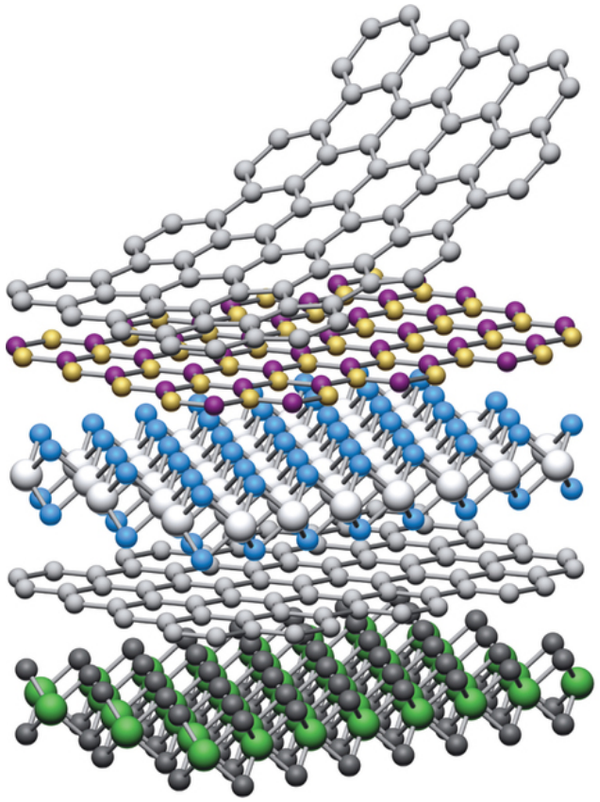
(E) Schematic view of the device in (D).

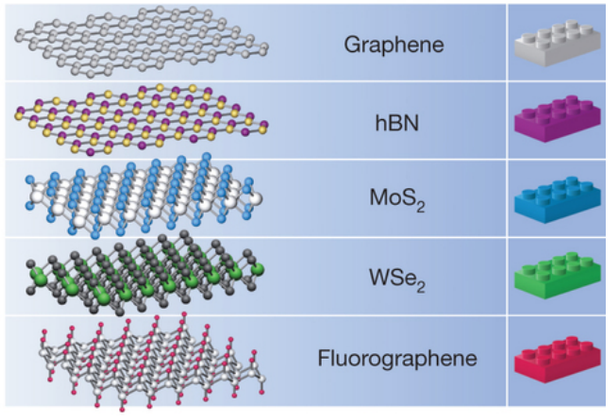


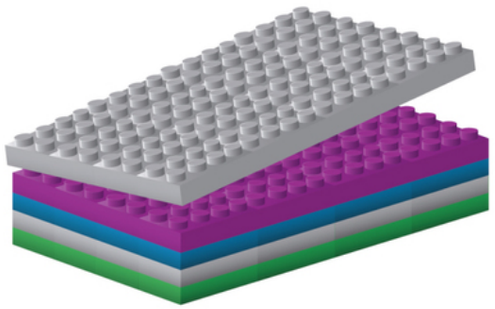
The 2000 Ig Nobel Prize in physics was awarded to Andre Geim, Radboud University Nijmegen, and Michael Berry, University of Bristol, UK, for the magnetic levitation of a live frog. Geim was awarded an actual Nobel Prize in Physics in 2010.[1]

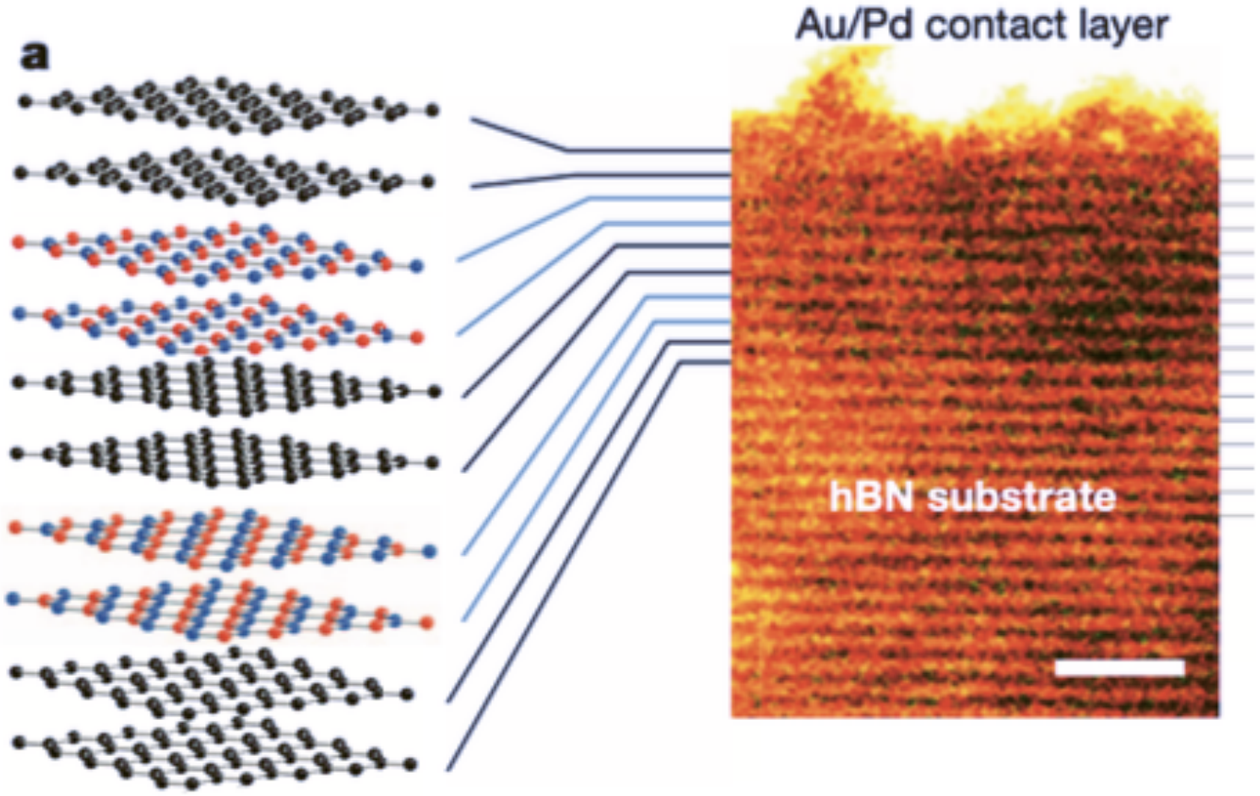


ساختارهای ناهمگون

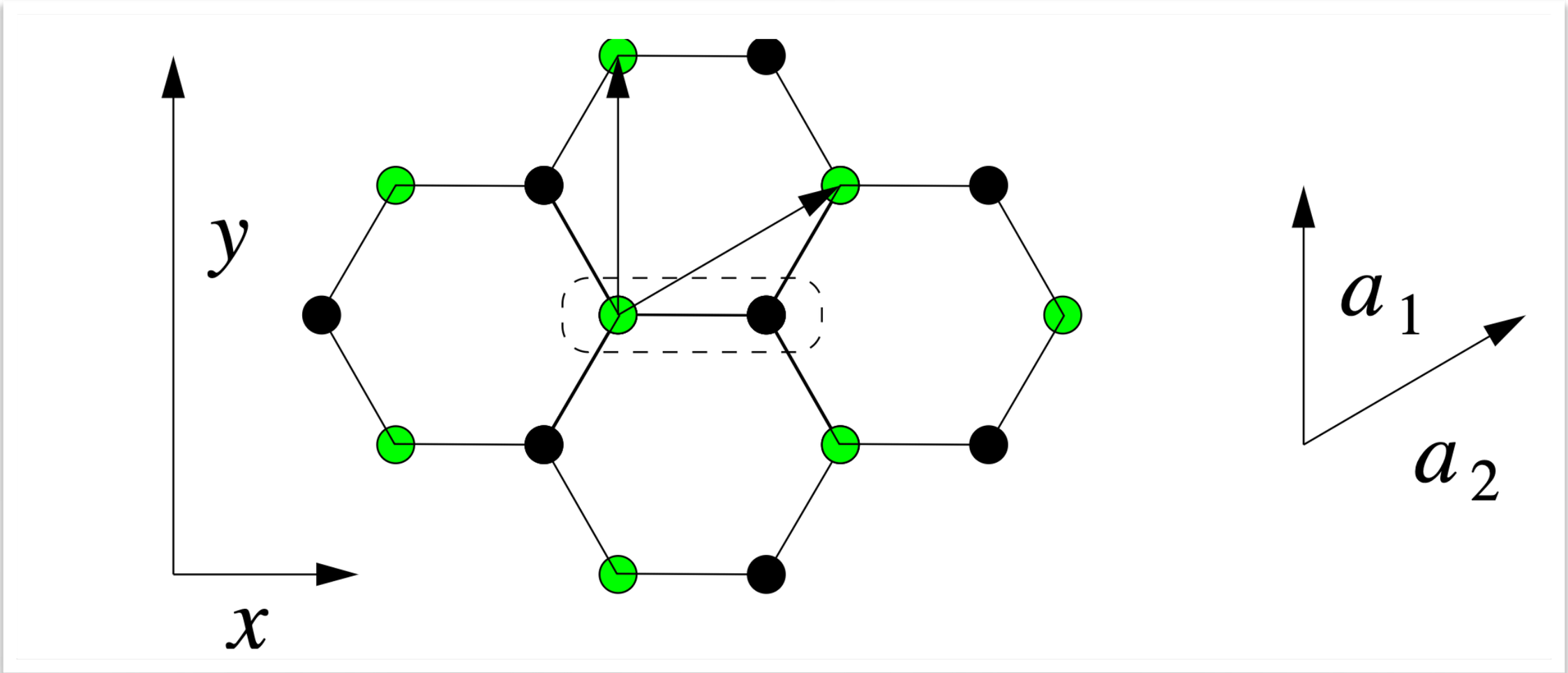








ساختار گرافین

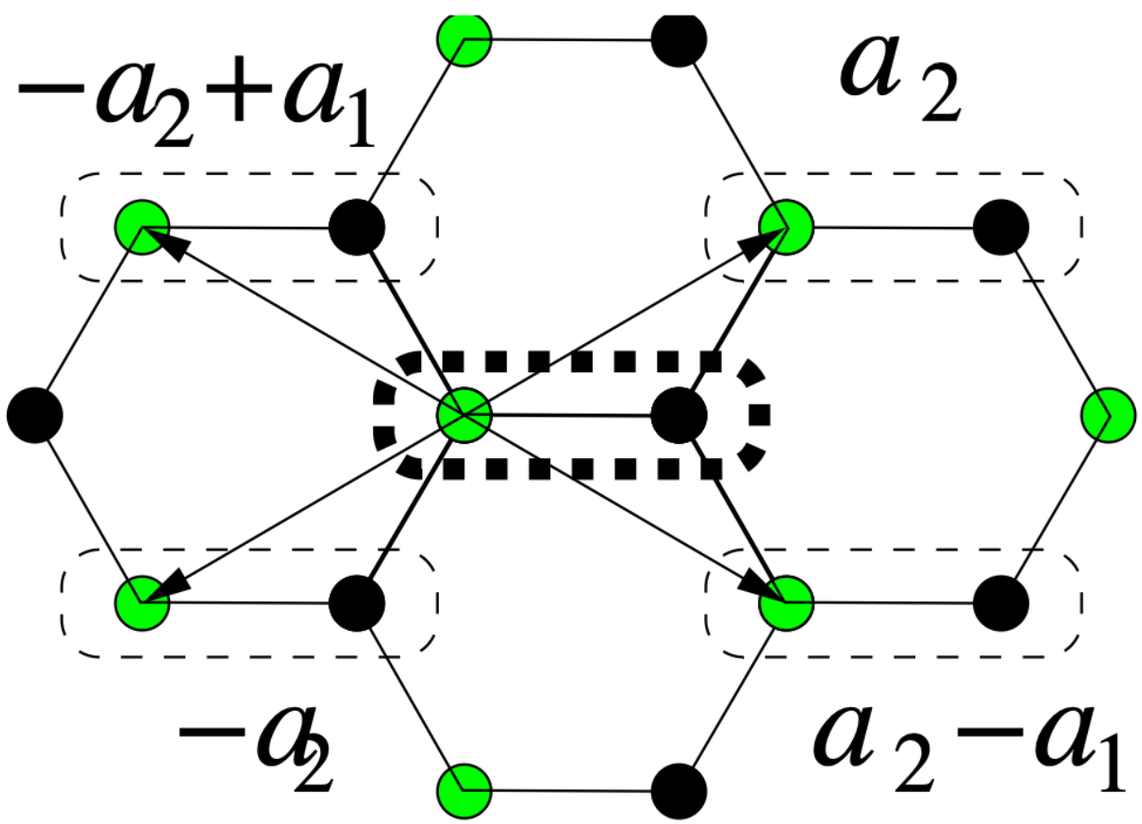


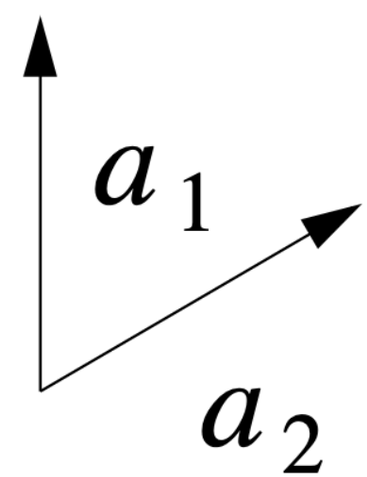
$$\begin{cases} \vec{a}_1 = a_0\,\hat{y} \\ \\ \vec{a}_2 = a_0\,\left(\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}\right) \end{cases}$$

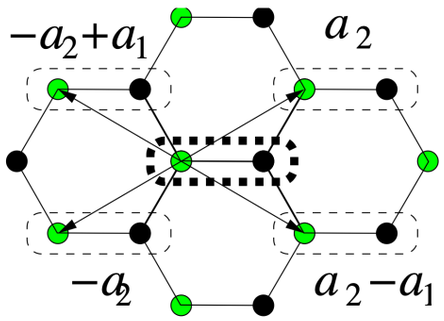
روش تنگابست

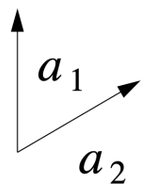
$$|\psi_{\vec{k}}\rangle = \frac{1}{N^{1/2}} \sum_{\vec{R}} \sum_{n=1}^{2} \mathrm{e}^{i\vec{k}\cdot\vec{R}} A_n^{\vec{k}} |\vec{R}\, n\rangle$$

$$\boxed{E(\vec{k}) A_{n'}^{\vec{k}} = \sum_{\vec{R}} \sum_{n}^{2} \mathrm{e}^{i\vec{k}\cdot(\vec{R}-\vec{R}')} A_n^{\vec{k}} \langle \vec{R}'\, n' | H | \vec{R}\, n\rangle}$$

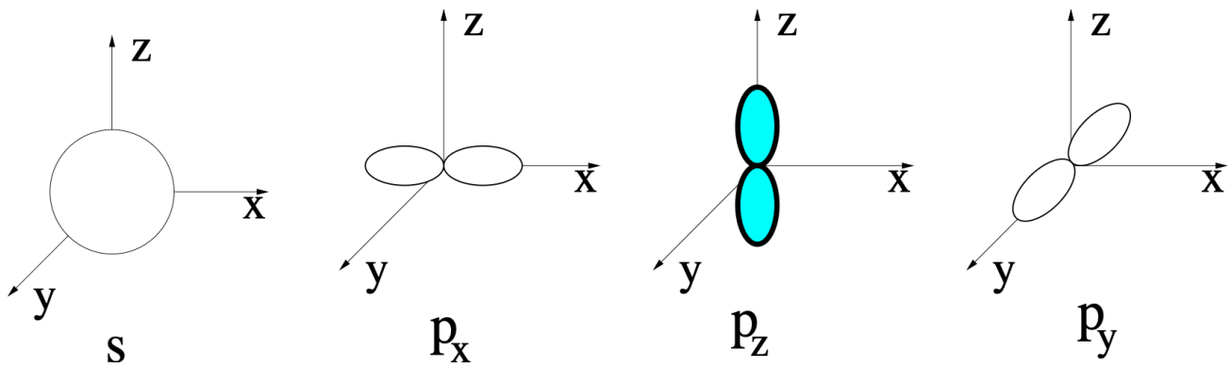








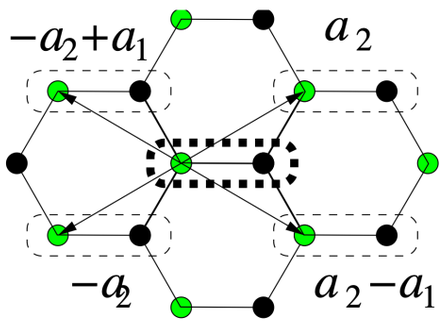
$$E(\vec{k})A^{\vec{k}}_{n'} = \sum_{\vec{R}}\sum_{n}^{2} \mathrm{e}^{i\vec{k}\cdot(\vec{R}-\vec{R}')} A^{\vec{k}}_{n}\langle \vec{R}'\, n'|H|\vec{R}\, n\rangle$$

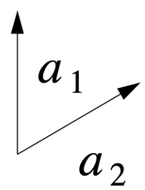


On-site energy: coupling with the primitive cell

$$\langle \vec{R}'\, n'|H|\vec{R}'\, n\rangle = \begin{pmatrix} \epsilon_p & \gamma_{pp\pi} \\ \gamma_{pp\pi} & \epsilon_p \end{pmatrix}$$

The phase factor is $\mathrm{e}^{i\vec{k}\cdot(\vec{R}'-\vec{R}')} = 1$





$$E(\vec{k})A^{\vec{k}}_{n'} = \sum_{\vec{R}}\sum_{n}^{2} \mathrm{e}^{i\vec{k}\cdot(\vec{R}-\vec{R}')} A^{\vec{k}}_{n}\langle \vec{R}'\, n'|H|\vec{R}\, n\rangle$$

Off-diagonal terms: coupling with other cells

1. Cell $\vec{a}_2$

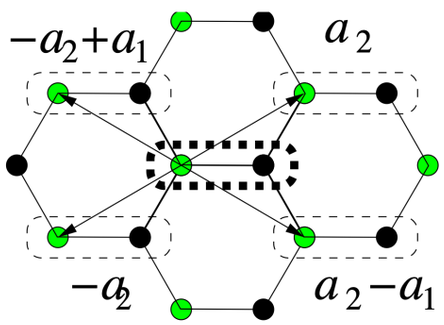
$$\langle \vec{R}'\, n'|H|\vec{R}' + \vec{a}_2\, n\rangle = \begin{pmatrix} 0 & 0 \\ \gamma_{pp\pi} & 0 \end{pmatrix}$$

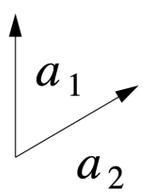
The phase factor is $\mathrm{e}^{i\vec{k}\cdot(\vec{R}'+\vec{a}_2-\vec{R}')} = \mathrm{e}^{i\vec{k}\cdot\vec{a}_2}$

2. Cell $\vec{a}_2 - \vec{a}_1$

$$\langle \vec{R}'\, n'|H|\vec{R}' + \vec{a}_2 - \vec{a}_1\, n\rangle = \begin{pmatrix} 0 & 0 \\ \gamma_{pp\pi} & 0 \end{pmatrix}$$

The phase factor is $\mathrm{e}^{i\vec{k}\cdot(\vec{R}'+\vec{a}_2-\vec{a}_1-\vec{R}')} = \mathrm{e}^{i\vec{k}\cdot(\vec{a}_2-\vec{a}_1)}$





$$E(\vec{k})A^{\vec{k}}_{n'} = \sum_{\vec{R}}\sum_{n}^{2} \mathrm{e}^{i\vec{k}\cdot(\vec{R}-\vec{R}')} A^{\vec{k}}_{n}\langle \vec{R}'\, n'|H|\vec{R}\, n\rangle$$

Off-diagonal terms: coupling with other cells

3. Cell $-\vec{a}_2$

$$\langle \vec{R}'\, n'|H|\vec{R}' - \vec{a}_2\, n\rangle = \begin{pmatrix} 0 & \gamma_{pp\pi} \\ 0 & 0 \end{pmatrix}$$

The phase factor is $\mathrm{e}^{i\vec{k}\cdot(\vec{R}'-\vec{a}_2-\vec{R}')} = \mathrm{e}^{-i\vec{k}\cdot\vec{a}_2}$

4. Cell $-\vec{a}_2 + \vec{a}_1$

$$\langle \vec{R}'\, n'|H|\vec{R}' - \vec{a}_2 + \vec{a}_1\, n\rangle = \begin{pmatrix} 0 & \gamma_{pp\pi} \\ 0 & 0 \end{pmatrix}$$

The phase factor is $\mathrm{e}^{i\vec{k}\cdot(\vec{R}'-\vec{a}_2+\vec{a}_1-\vec{R}')} = \mathrm{e}^{-i\vec{k}\cdot(\vec{a}_2-\vec{a}_1)}$

محاسبه ویژه مقادیر

$$E(\vec{k})A^{\vec{k}}_{n'} = \sum_{\vec{R}}\sum_{n}^{2} \mathrm{e}^{i\vec{k}\cdot(\vec{R}-\vec{R}')} A^{\vec{k}}_{n} \langle \vec{R}'\, n' | H | \vec{R}\, n \rangle$$

$$E(\vec{k})\Psi_{\vec{k}} = \begin{pmatrix} \epsilon_p & \gamma_{pp\pi}\, f(\vec{k}) \\ \gamma_{pp\pi}\, f(\vec{k})^* & \epsilon_p \end{pmatrix} \Psi_{\vec{k}}$$

$$f(\vec{k}) = 1 + \mathrm{e}^{-i\vec{k}\cdot\vec{a}_2} + \mathrm{e}^{-i\vec{k}\cdot(\vec{a}_2-\vec{a}_1)} \ = 1 + 2\,\mathrm{e}^{-ik_x\frac{\sqrt{3}}{2}a_0}\cos(\frac{k_y}{2}a_0)$$

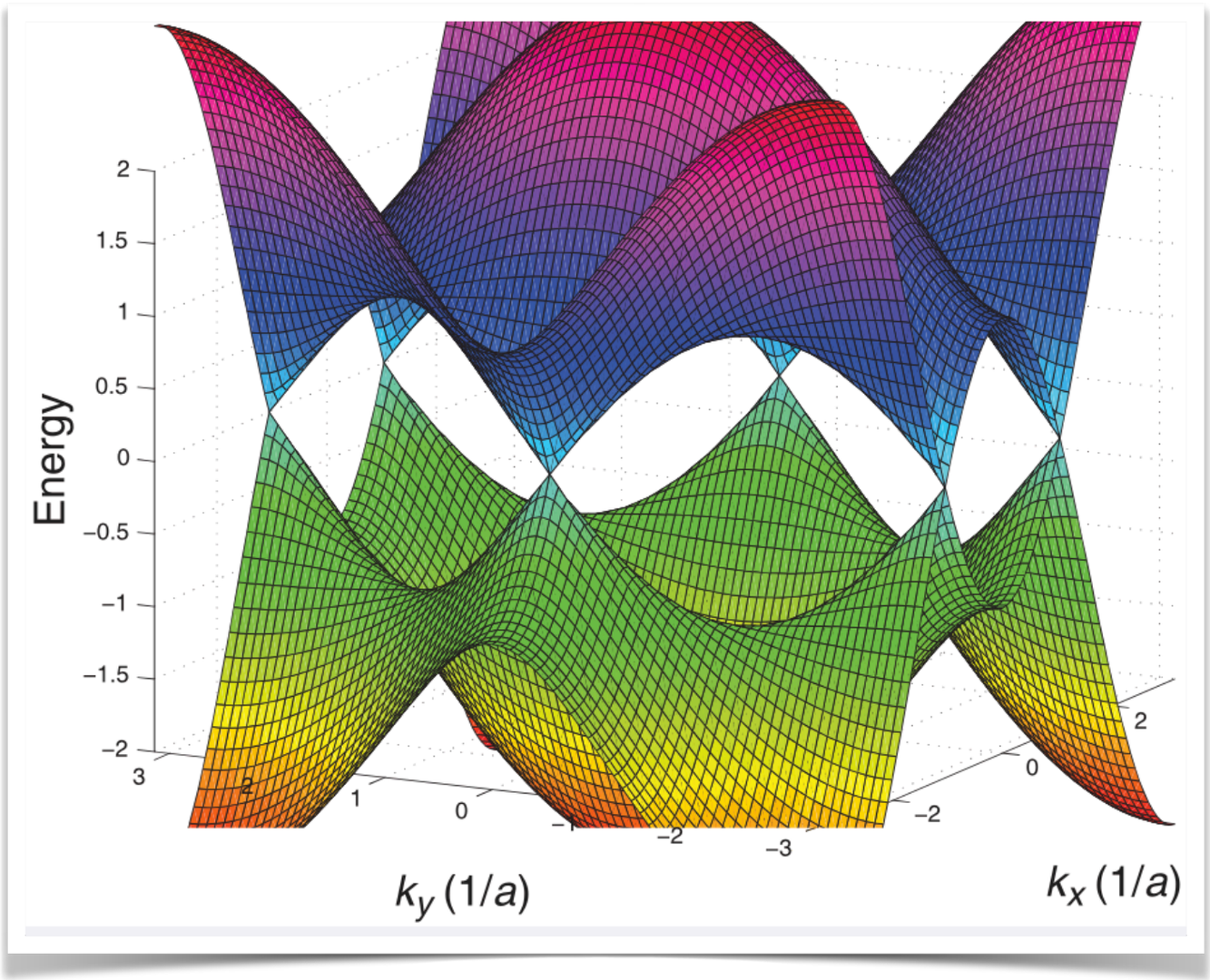
$$\det\begin{pmatrix} \epsilon_p - E(\vec{k}) & \gamma_{pp\pi}\, f(\vec{k}) \\ \gamma_{pp\pi}\, f(\vec{k})^* & \epsilon_p - E(\vec{k}) \end{pmatrix} = 0$$

$$E(\vec{k}) = \epsilon_p \pm \gamma_{pp\pi}\sqrt{f(\vec{k})f(\vec{k})^*}$$

ساختار نواری

$$E(\vec{k}) = \epsilon_p \pm$$

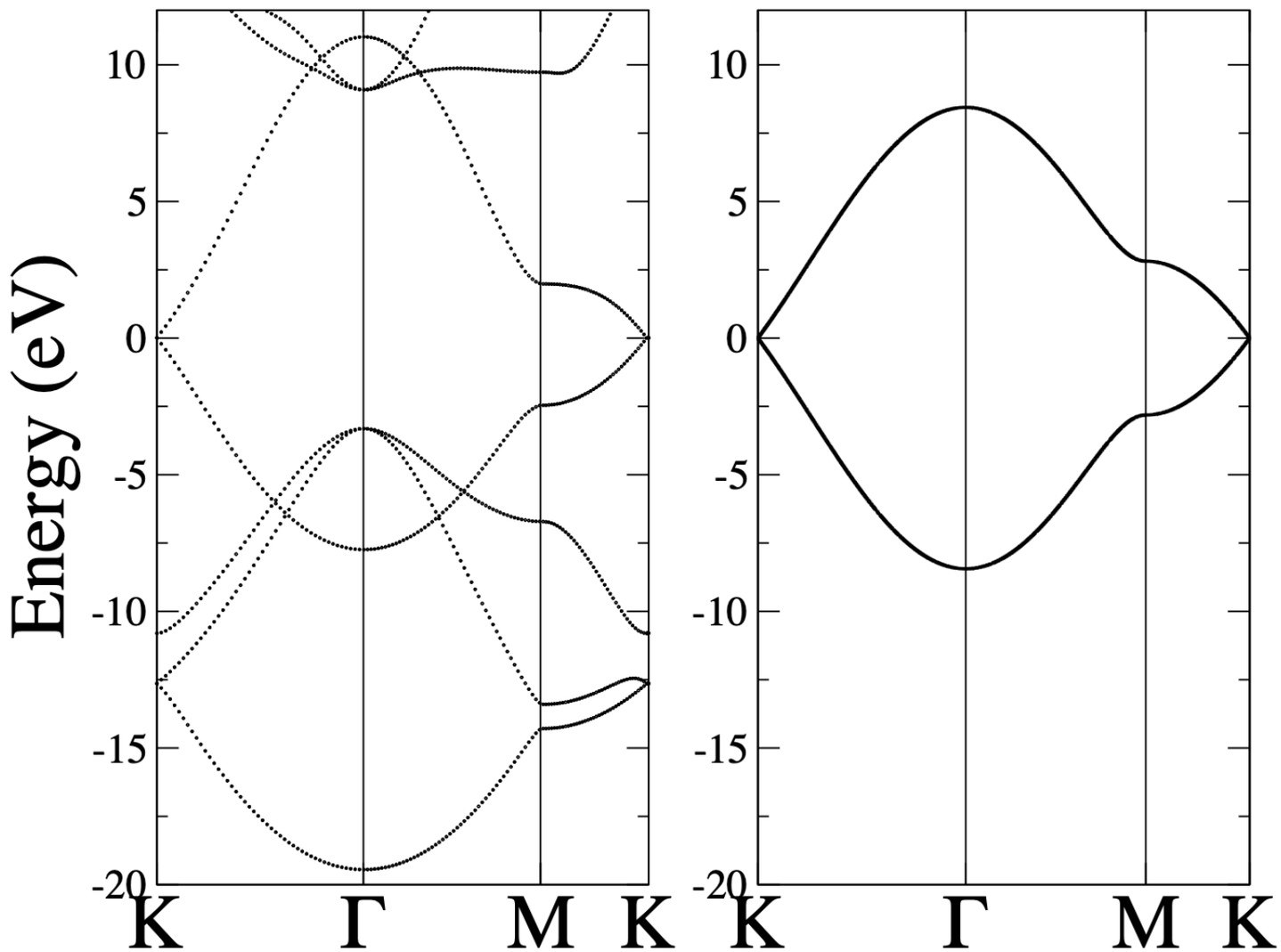
$$\pm\gamma_{pp\pi}\sqrt{1 + 4\cos^2\left(\frac{k_y a_0}{2}\right) + 4\cos\left(\frac{k_y a_0}{2}\right)\cos\left(\frac{\sqrt{3}}{2}k_x a_0\right)}$$



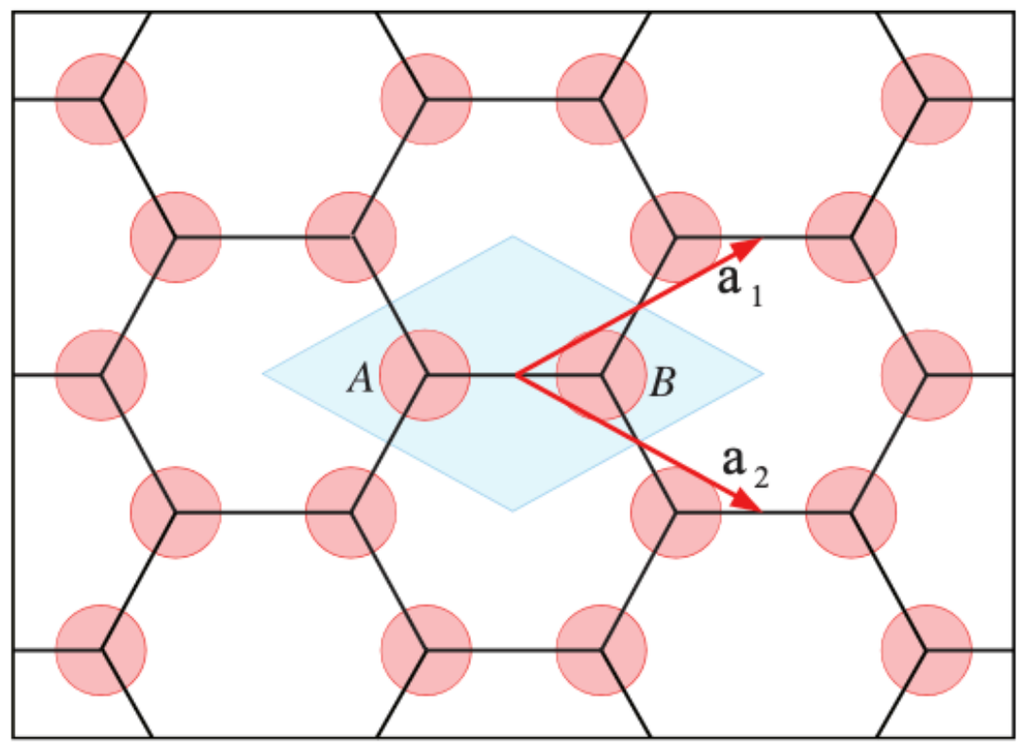
ساختار نواری

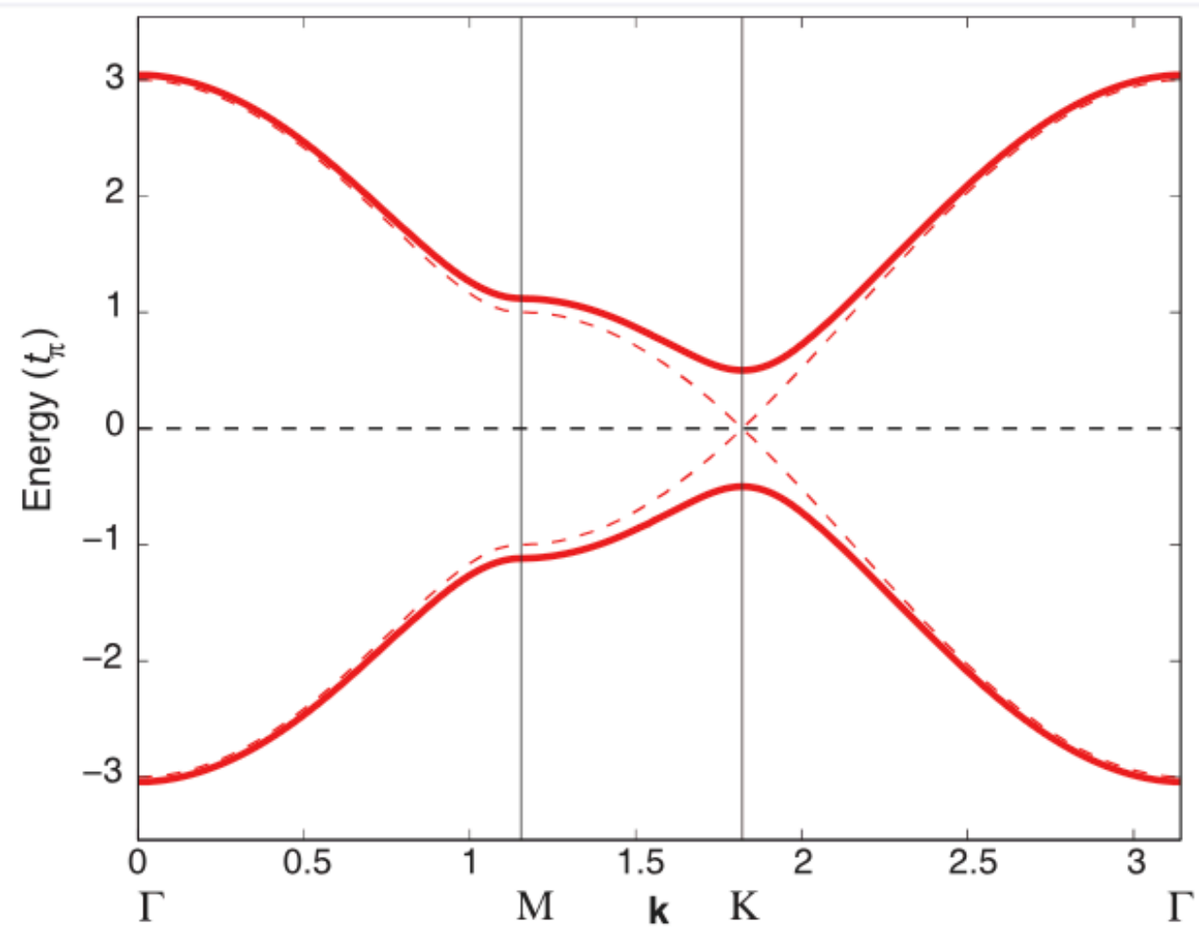
$$E(\vec{k}) = \epsilon_p \pm$$

$$\pm\gamma_{pp\pi}\sqrt{1 + 4\cos^2\left(\frac{k_y a_0}{2}\right) + 4\cos\left(\frac{k_y a_0}{2}\right)\cos\left(\frac{\sqrt{3}}{2}k_x a_0\right)}$$



پروژه : اثر شکست تقارن وارونی بر ساختار نواری





مراحل انجام پروژه (تیم ۳ نفره)

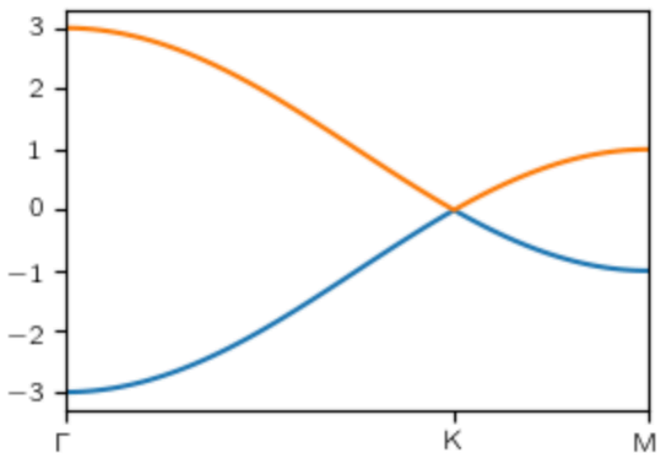
۱- مطالعه مقاله

۲- محاسبه ساختار نواری گرافین و h-BN با استفاده از روش تنگابست

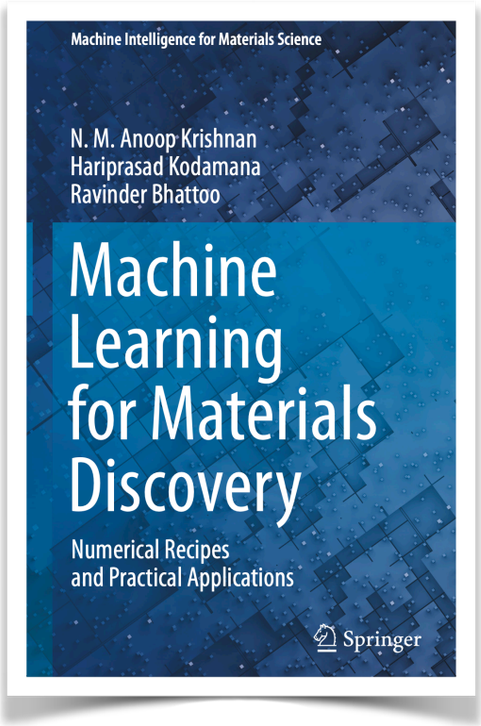
۳- محاسبه ساختار نواری گرافین و h-BN با استفاده از بسته محاسباتی PythTB

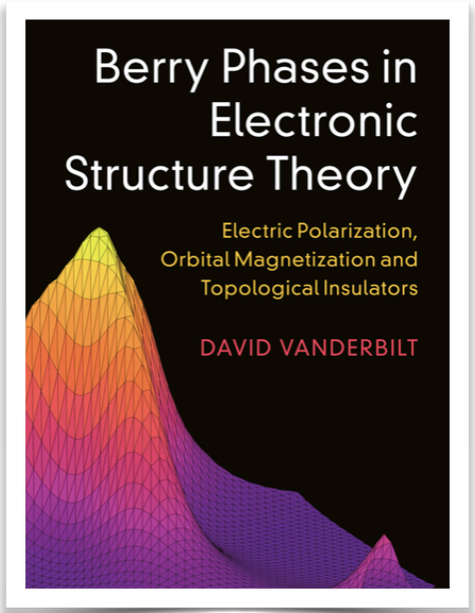
```
from pythtb import *

# lattice vectors and orbital positions
lat=[[1.0, 0.0], [0.5, np.sqrt(3.0)/2.0]]
orb=[[1./3., 1./3.], [2./3., 2./3.]]

# two-dimensional tight-binding model
gra=tb_model(2, 2, lat, orb)

# define hopping between orbitals
gra.set_hop(-1.0, 0, 1, [ 0, 0])
gra.set_hop(-1.0, 1, 0, [ 1, 0])
gra.set_hop(-1.0, 1, 0, [ 0, 1])

# solve model on a path in k-space
k=[[0.0, 0.0],[1./3., 2./3.],[0.5,0.5]]
(k_vec,k_dist,k_node)=gra.k_path(k, 100)
evals=gra.solve_all(k_vec)

# plot bandstructure
import matplotlib.pyplot as plt
fig, ax = plt.subplots()
ax.plot(k_dist,evals[0,:])
ax.plot(k_dist,evals[1,:])
ax.set_xticks(k_node)
ax.set_xticklabels(["$\Gamma$","K","M"])
ax.set_xlim(k_node[0],k_node[-1])
fig.savefig("band.png")
```

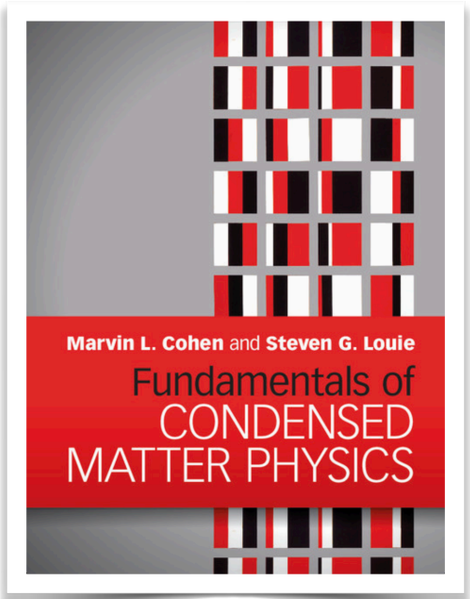
۴- بررسی شکست تقارن وارونی

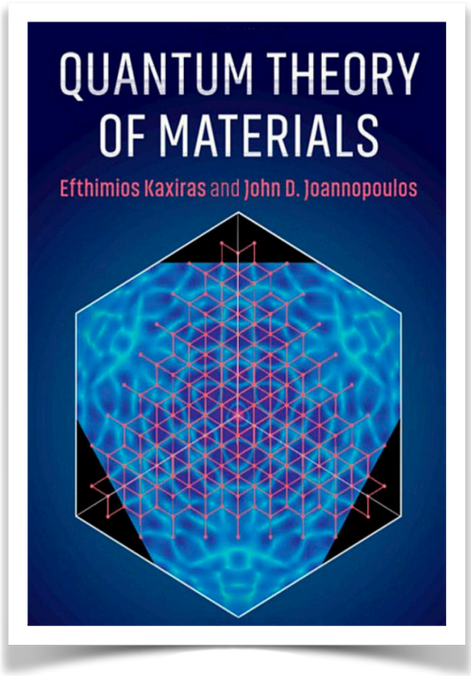


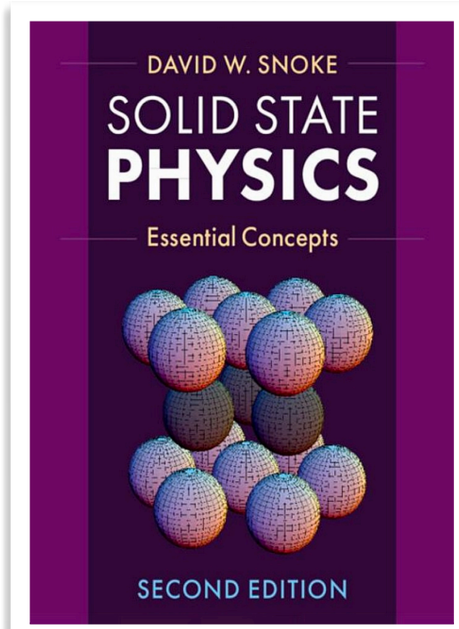
مراجع

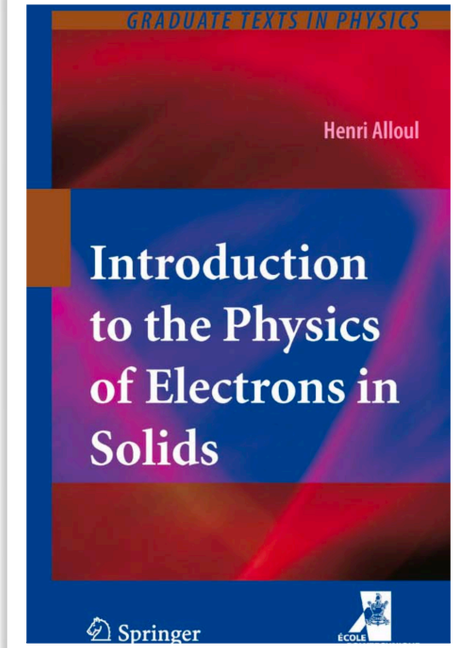












Stefano Sanvito Lecture note

PHYSICAL REVIEW B **93**, 085424 (2016)

Highly anisotropic thermal conductivity of arsenene: An *ab initio* study

Majid Zeraati,[1] S. Mehdi Vaez Allaei,[1,2,*] I. Abdolhosseini Sarsari,[3] Mahdi Pourfath,[4,5] and Davide Donadio[6,7,8,9,†]

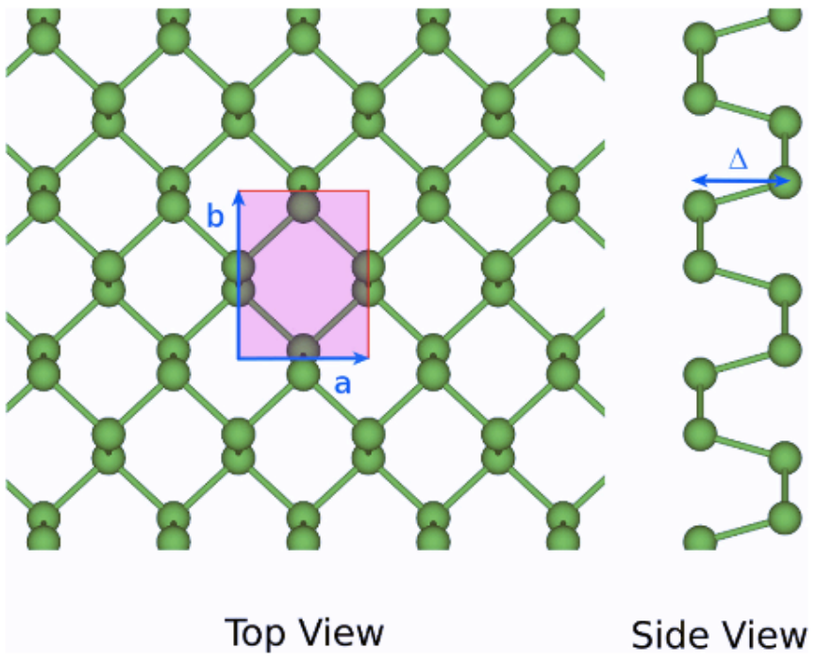
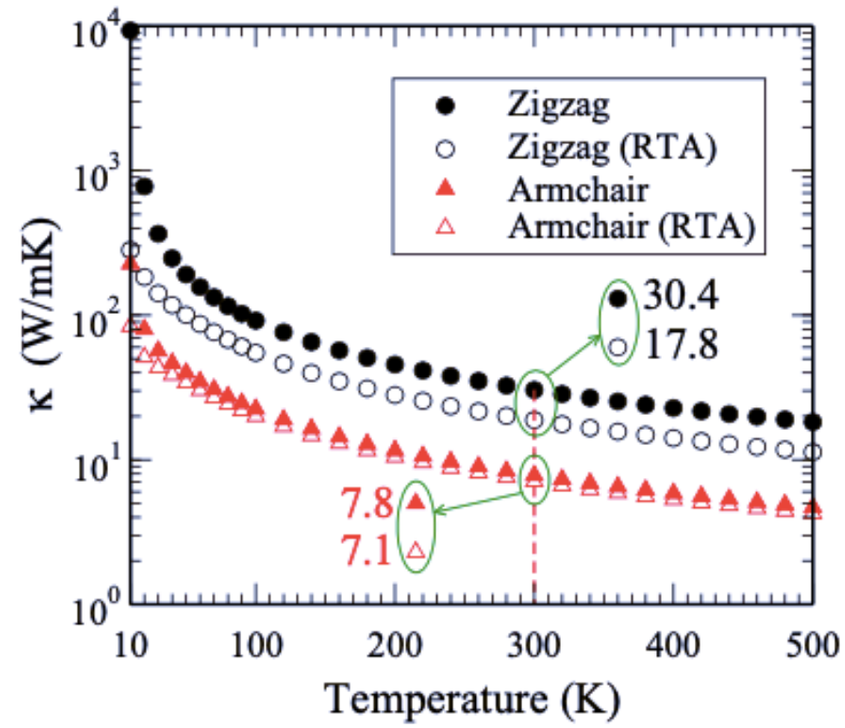


FIG. 1. Top and side views of puckered arsenene.



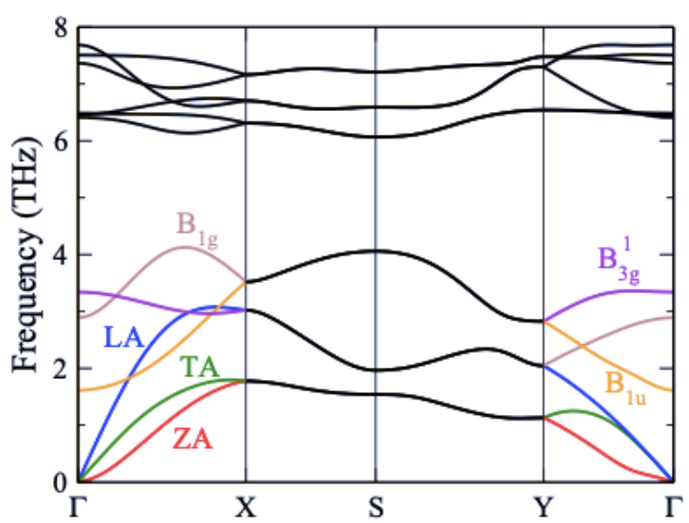
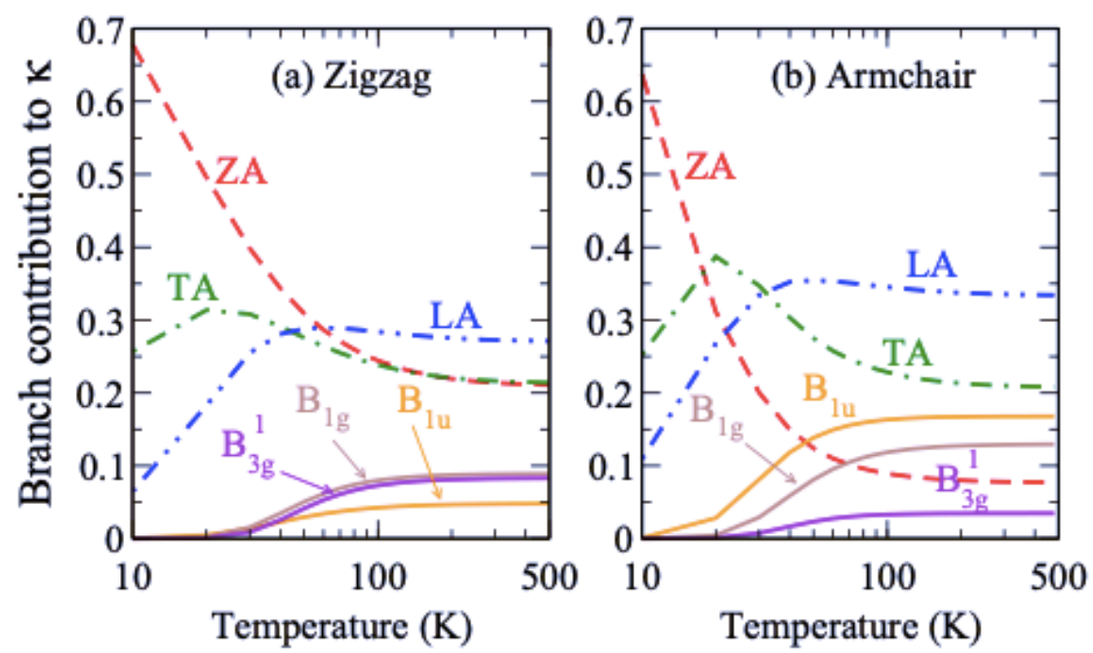


FIG. 2. Phonon dispersion curves along the high-symmetry directions of the first Brillouin zone for puckered arsenene.



PAPER

Electronic and interfacial properties of graphene/HfS_2 van der Waals heterostructure

S Karbasizadeh, F Fanaeeparvar and I Abdolhosseini Sarsari
Department of Physics, Isfahan University of Technology, Isfahan 84156-83111, Iran
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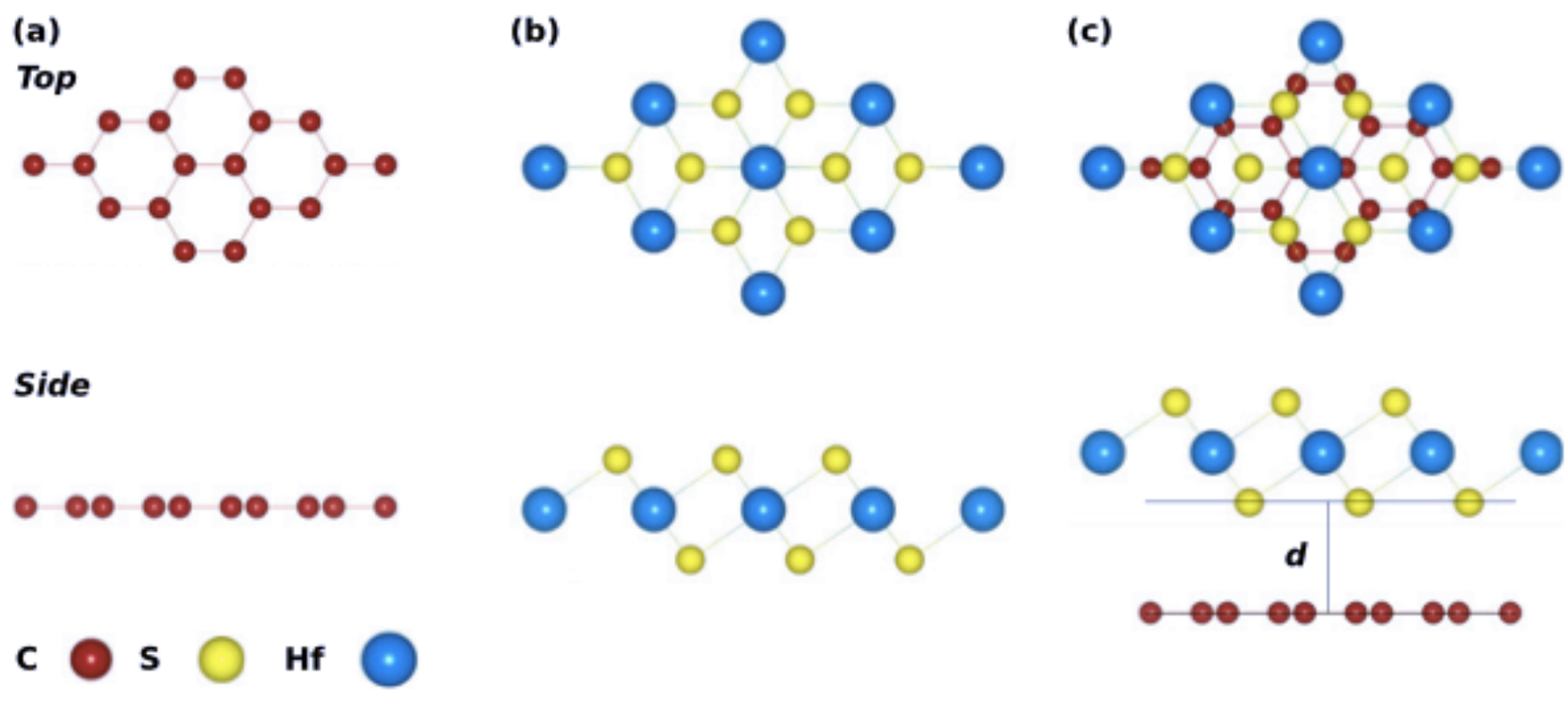

Figure 2. Schematic graphics of optimized crystalline structures of (a) 3 × 3 × 1 supercell of graphene, (b) 2 × 2 × 1 supercell of HfS_2 and (c) G/HfS_2 vdW heterostructure.

PHYSICAL REVIEW B **102**, 134103 (2020)

Theoretical study of quantum emitters in two-dimensional silicon carbide monolayers

Q. Hassanzada,[1] I. Abdolhosseini Sarsari,[1] A. Hashemi,[2] A. Ghojavand,[1] A. Gali,[3] and M. Abdi[1]
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[2]*Department of Applied Physics, Aalto University, FI-00076 Aalto, Finland*
[3]*Department of Atomic Physics, Budapest University of Technology and Economics, Budafoki út 8, 1111 Budapest, Hungary*

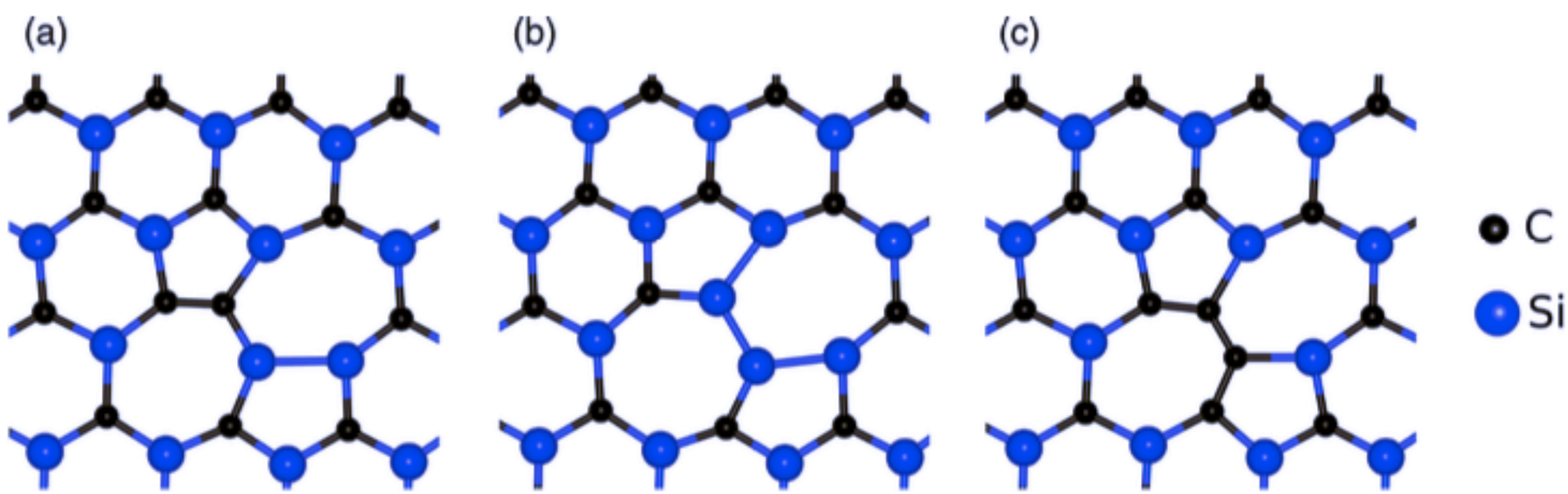
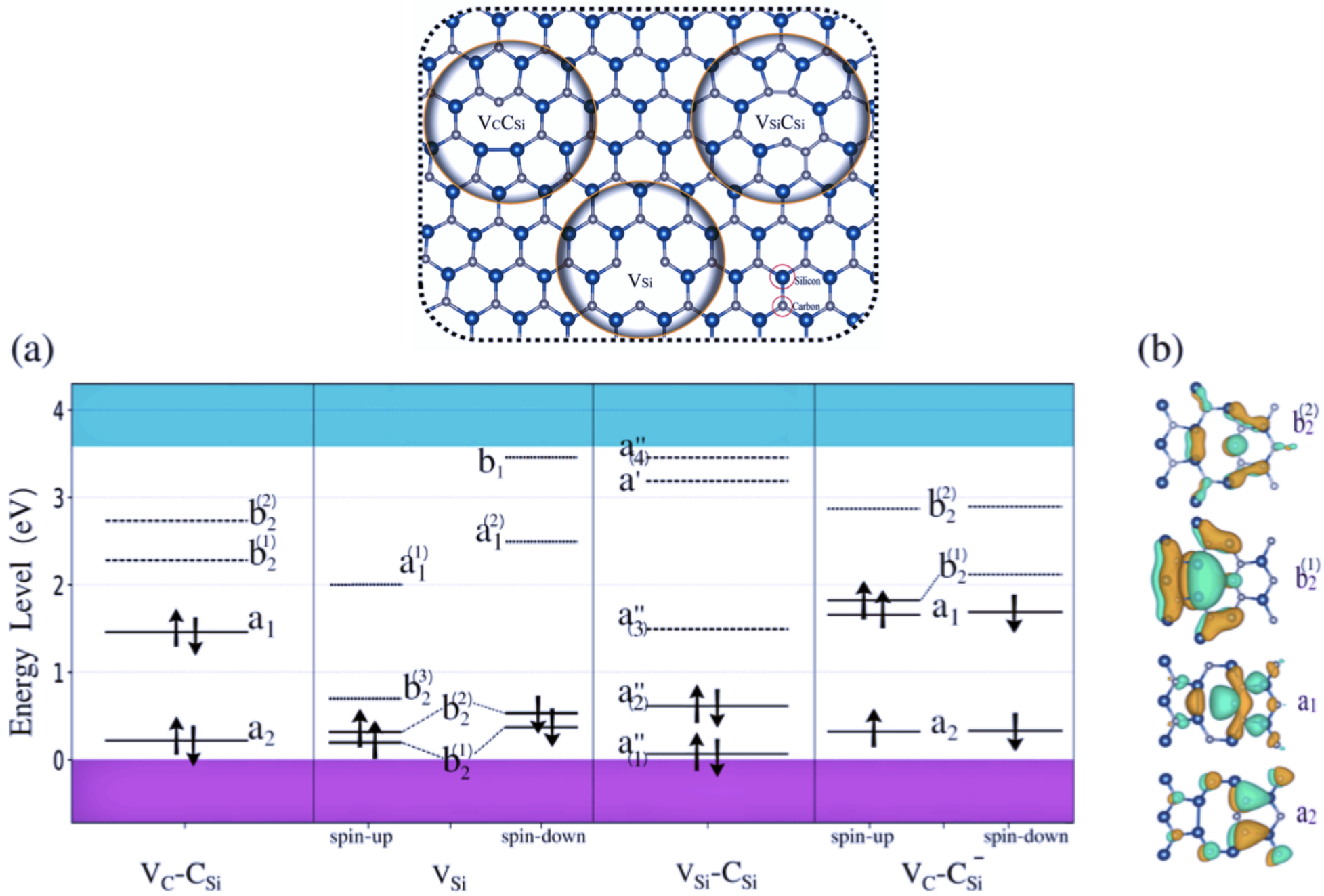


FIG. 1. Atomic structure of (a) SW, (b) SW-Si_C, and (C) SW-C_{Si} defects. Silicon and carbon atoms are illustrated by blue and black colors, respectively

PHYSICAL REVIEW MATERIALS **8**, 056201 (2024)

Vacancy-related color centers in two-dimensional silicon carbide monolayers

M. Mohseni,[1,2,3] I. Abdolhosseini Sarsari,[3,*] S. Karbasizadeh,[3] Péter Udvarhelyi,[1,4] Q. Hassanzada,[5] T. Ala-Nissila,[6,7] and A. Gali[1,4,8,†]



Quantum Science and Technology

PAPER

Strain induced coupling and quantum information processing with hexagonal boron nitride quantum emitters

F T Tabesh[1], Q Hassanzada[1,2], M Hadian[1], A Hashemi[3], I Abdolhosseini Sarsari[1] and M Abdi[1,*]

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[3] Department of Applied Physics, Aalto University, PO Box 11100, 00076 Aalto, Finland
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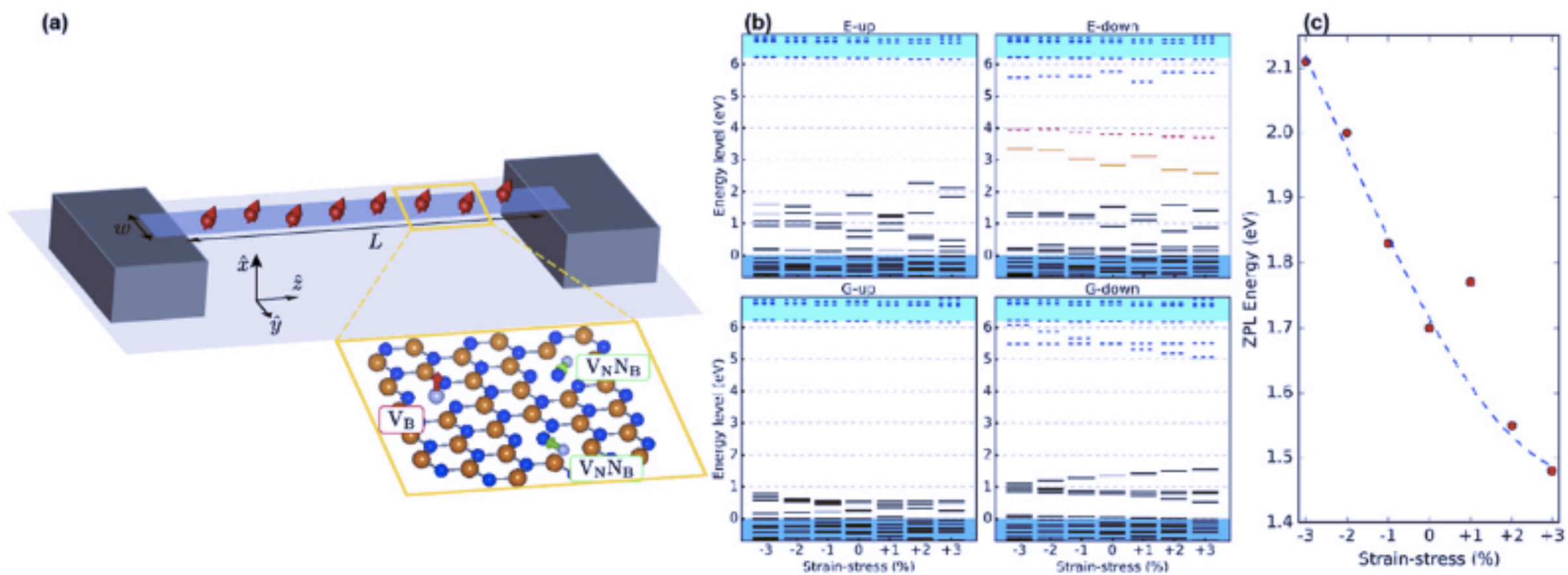
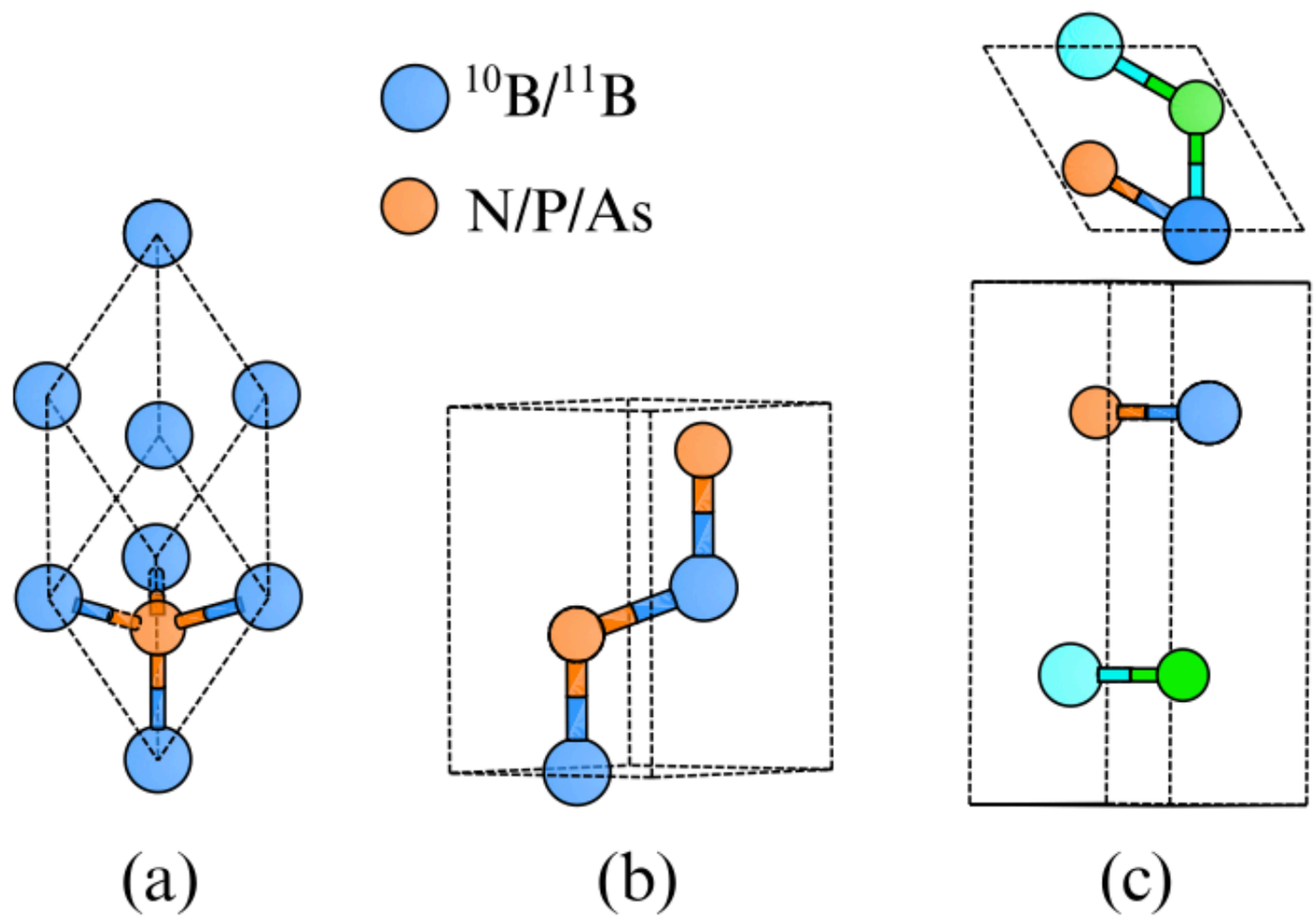


PHYSICAL REVIEW B **111**, 205204 (2025)

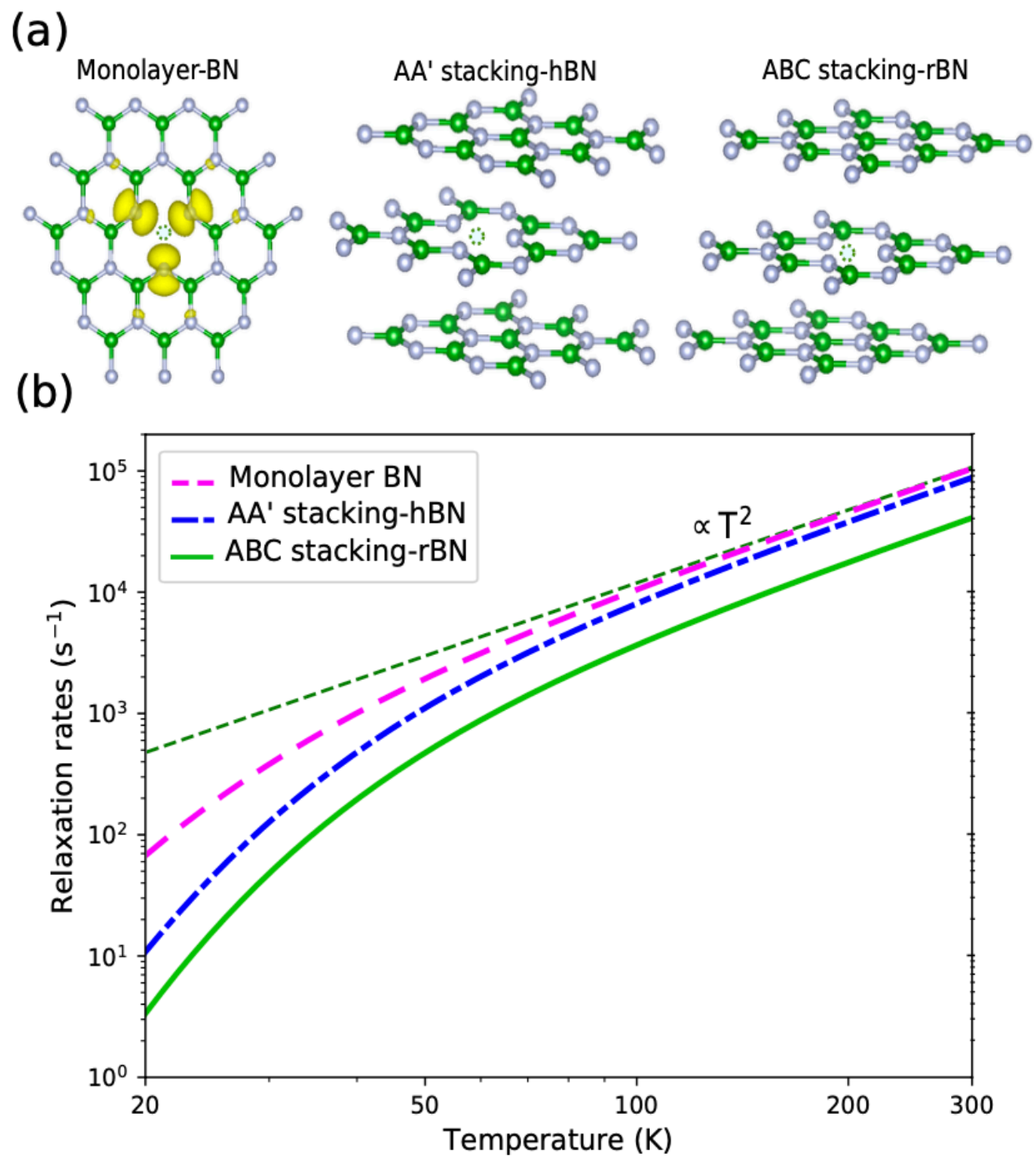
Boron isotope effects on Raman scattering in bulk BN, BP, and BAs: A density functional theory study

Nima Ghafari Cherati,[1,2] I. Abdolhosseini Sarsari,[3] Arsalan Hashemi,[4,*] and Tapio Ala-Nissila[4,5,†]



Spin-Phonon Relaxation of Boron-Vacancy Centers in Two-Dimensional Boron Nitride Polytypes

Nasrin Estaji,[1] Ismaeil Abdolhosseini Sarsari,[1] Gergő Thiering,[2] and Adam Gali[2,3,4,*]



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