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Courses » Solid State Chemistry

Announcements

Course

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Unit 14 - Week 11 : Theory of Electronic Structure of Solids

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Course outline

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Practice

Week 1 : Solid
State And Solid
State Materials

Week 2 Unit
Cells And
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Week 3 :
Symmetry In
Crystals Part 1

Week 4 :
Symmetry in
Crystals Part 2

Week 5 : Crystal
Systems, Point
Groups and
Space Groups

Week 6 :
Crystallographic
Notations

Week 7 :
Coordination
number, voids,
defects in

Assignment 11

The due date for submitting this assignment has passed.

As per our records you have not submitted this assignment. **Due on 2019-04-17, 23:59 IST.**

1) For a free electron in 3 dimensions travelling along the negative z direction, the wavefunction **1 point** in the usual notation is given by (here k is a component of the wavevector)

e^{ikz}

e^{-ikz}

$e^{-ik(x+y+z)}$

$e^{ik(x+y+z)}$

No, the answer is incorrect.

Score: 0

Accepted Answers:

e^{-ikz}

2) For an electron in 3 dimensions confined to a cubic box of length L located between $x = 0$ and $x = L$, $y = 0$ and $y = L$ and $z = 0$ and $z = L$, the wavefunction is proportional to (here n_x , n_y and n_z are positive integers) **1 point**

$\sin\left(\frac{(n_x+n_y+n_z)\pi x}{L}\right)$

$\sin\left(\frac{n_x\pi x}{L}\right) \sin\left(\frac{n_y\pi y}{L}\right) \sin\left(\frac{n_z\pi z}{L}\right)$

$\sin\left(\frac{(n_x+n_y+n_z)\pi(x+y+z)}{L}\right)$

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Concepts related to X-ray Diffraction

Week 9 : X - Ray Diffraction, X - Ray Crystallography & Electron Microscopy

Week 10 : Common Crystal Structures

Week 11 : Theory of Electronic Structure of Solids

- Lecture 51 : Free electron Models
- Lecture 52 : Bloch Theorem
- Lecture 53 : Band Theory of Solids
- Lecture 54 : Bands in Higher Dimensions
- Lecture 55 : Summary of Week 11 and Practice Problems
- Quiz : Assignment 11
- Feedback For Week 11
- Assignment 11 Solution

Interaction Session

Week 12 : Theory of Electronic Structure of Solids, Part 2

3) For a system of 20 electrons in 2 dimensions confined to cubic box of length L located between $x = 0$ and $x = L, y = 0$ and $y = L$, the Fermi energy is equal to **1 point**



$$\frac{5h^2}{m_e L^2}$$



$$\frac{17h^2}{m_e L^2}$$



$$\frac{32h^2}{m_e L^2}$$



None of the other choices

No, the answer is incorrect.

Score: 0

Accepted Answers:

None of the other choices

4) The effect of lattice periodicity on the wavefunction of a Bloch electron is given by the condition (here \vec{R} is the Bravais lattice translation vector and \vec{K} is the reciprocal lattice translation vector) **1 point**



$$\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k}}(\vec{r} + \vec{R})$$



$$\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k} + \vec{K}}(\vec{r})$$



$$\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k} + \vec{K}}(\vec{r} + \vec{R})$$



None of the other choices

No, the answer is incorrect.

Score: 0

Accepted Answers:

$$\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k} + \vec{K}}(\vec{r})$$

5) Bloch's theorem assumes that the valence electrons of the metal **1 point**



do not interact with each other



are confined within the crystal



experience a periodic potential due to the atoms



satisfy all the other three choices

No, the answer is incorrect.

Score: 0

Accepted Answers:

satisfy all the other three choices

6) The Born- von Karman boundary conditions imply that the wave vector \vec{k} of the electron in a crystal satisfies (Here \vec{R} and \vec{K} are translation vectors of the Bravais lattice and the reciprocal lattice respectively) **1 point**



$$e^{i\vec{k}\vec{R}} = 1$$



$$e^{i\vec{k}\vec{R}} = e^{i(\vec{k} + \vec{K})\vec{R}}$$



$\vec{k} = \frac{n_x\pi}{L_x}\hat{i} + \frac{n_y\pi}{L_y}\hat{j} + \frac{n_z\pi}{L_z}\hat{k}$ where L_x, L_y, L_z are the lengths of the cell in the three directions and n_x, n_y, n_z are integers



None of the other choices

No, the answer is incorrect.

Score: 0

Accepted Answers:

$\vec{k} = \frac{n_x\pi}{L_x}\hat{i} + \frac{n_y\pi}{L_y}\hat{j} + \frac{n_z\pi}{L_z}\hat{k}$ where L_x, L_y, L_z are the lengths of the cell in the three directions and n_x, n_y, n_z are integers

7) For a 1D lattice of size a in a crystal of size L , the separation between allowed values of the wave vector k is equal to **1 point**



$2\pi/a$



$2\pi/L$



π/L



None of the other choices

No, the answer is incorrect.

Score: 0

Accepted Answers:

π/L

8) The concept of band gap is illustrated by **1 point**



the free electron model



the free electron model with the constraint of lattice periodicity



the nearly free electron model where the electron interacts weakly with the periodic lattice



None of the other choices

No, the answer is incorrect.

Score: 0

Accepted Answers:

the nearly free electron model where the electron interacts weakly with the periodic lattice

9) The effect of lattice periodicity on the energy of a Bloch electron is given by the relation **1 point**



$E(\vec{r}) = E(\vec{r} + \vec{R})$ only if \vec{R} is a Bravais lattice vector



$E_{\vec{k}} = E_{\vec{k}+\vec{K}}$ only if \vec{K} is a reciprocal lattice vector



$E_{\vec{K}} = 0$ only if \vec{K} is a reciprocal lattice vector



None of the other choices

No, the answer is incorrect.

Score: 0

Accepted Answers:

$E_{\vec{k}} = E_{\vec{k}+\vec{K}}$ only if \vec{K} is a reciprocal lattice vector

10) The first Brillouin zone of a monoatomic BCC crystal has the shape of a **1 point**

- cube
- truncated octahedron
- rhombic dodecahedron
- None of the other choices

No, the answer is incorrect.

Score: 0

Accepted Answers:

rhombic dodecahedron



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