

Indian Institute of Information Technology Allahabad

Materials Informatics Assignment

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Submission Date 19/04/2024

Q1. Explain Density Functional Theory? How DFT work in finding the electronic structure and density of state?

Q2. Explain the meaning of Functional in DFT with different suitable example.

Q3. Define the Following Terminology and write the equation.

- (i) Coulomb Potential
- (ii) Hartree-Fock
- (iii) Hohenberg-Kohn theorem
- (iv) Kohn-Sham Equation

Q4. What is exchange- correlation function? Give a suitable example of exchange correlation functional?

Q5. The De-Broglie wavelength of particles of mass m with average momentum p at a temperature T in one dimension is given by?

Q6. For the given wave function ($\psi(x) = Nxe^{-ix}$) calculate the N normalised constant and Probability of the wave function. The range of x lies $-L < x < L$?

Q7. Consider the one-dimensional wave function ($\psi(x) = A(x/x_0)^n e^{-x/x_0}$), where A , n and x_0 are constants. Using Schrodinger equation, find the potential $V(x)$ and energy E for which this wave function is an eigenfunction. (Assume that as $x \rightarrow \infty$, $V(x) \rightarrow 0$)?

Q8. Consider a particle in one- dimensional box whose length is $-L$ to L . Write down the 5th level of Energy?

Q9. A particle of mass m is confined in the ground state of a one-dimensional box, extending from $x = -2L$ to $x = +2L$. The wave function of the particle in this state is $\Psi(x) = \Psi_0 \cos(\pi x/4L)$, where Ψ_0 is constant. Calculate the normalization factor Ψ_0 of this wave length?

Q10. If the wave function of a particle trapped in space between $x = 0$ and $x = L$ is given by $\Psi(x) = A \sin(2\pi x/L)$, where A is a constant, for which value of x will the probability of finding the particle be the maximum?