

July 2, 2012

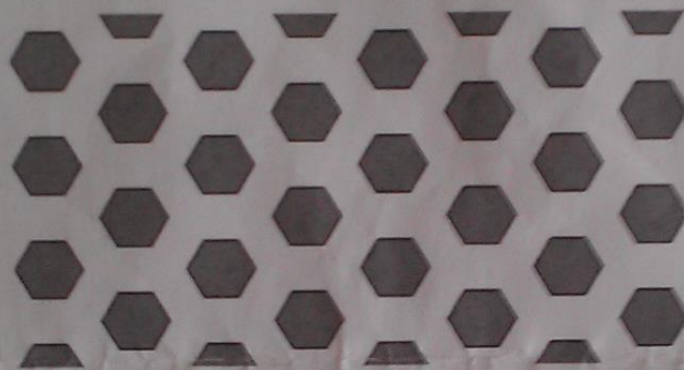
Problem 1: Molecular orbitals

An isolated carbon atom has two 2s electrons and two 2p electrons. When it forms methane CH_4 , it forms sp^3 hybrid orbitals where one of the 2s electrons gets promoted into the 2p shell. You could show that this decreases the total energy for the molecule by calculating the molecular orbitals. Write down the Hamiltonian and the wave function that you will need to calculate the molecular orbitals. Explain how to

calculate the energy of the molecular orbitals.

Problem 2: Fourier series

A two dimensional periodic function is defined such that it has a constant value c inside hexagons that are arranged on a hexagonal pattern and is zero outside the hexagons.



This periodic function can be written as a Fourier series,

$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}.$$

- How are the reciprocal lattice vectors \vec{G} determined?
- How are the structure factors $f_{\vec{G}}$ determined?

Problem 3: Equivalent planes

A crystal has a set of equivalent planes $\langle 100 \rangle$. Write down one of the symmetry elements of the point group for this crystal. The symmetry element is a 3×3 matrix. What consequences does this symmetry have for quantities like the conductivity or the electric susceptibility?

Problem 4: Polymer

A polymer can be considered to be a one dimensional crystal where the monomer is the unit cell. Draw approximately the electron dispersion (E vs. k) for a polymer. Most monomers have an even number of electrons. This is because molecules with an odd number of electrons are radicals and are chemically unstable. If there are an even number of electrons in the unit cell, is this a metal or an insulator? Explain your reasoning.