

Assignment P2-1

1. In the molecular surface reaction of N_2 interaction with iron (Fe) solid surface, the elemental iron is *bcc* in its ground state, which is metallic only due to 2 of its valence electrons. Within the free electron theory, calculate the Fermi energy (E_F in the units of eV) of elemental iron (Fe at $T = 0$ K). Consider the atomic radius of Fe is 1.86 \AA .

Plank constant (\hbar ; read it as h-bar) = $1.05 \times 10^{-34} \text{ J.s}$

Mass of electron (m) = $9.1 \times 10^{-31} \text{ kg}$

1 eV = $1.6 \times 10^{-19} \text{ J}$

2. Write the Hamiltonian that one would need to calculate the electronic wavefunction for a system of interacting particles. The system consisting of two atoms labeled as A and B each with an electron is pictorially depicted below.

