

Kittel.

3.3. $H_2: \epsilon = 50 \times 10^{-16}$ erg.

$\sigma = 2.96 \text{ \AA}$

cohesive energy in.
kJ/mole.

fcc.

treat each H_2 as sphere.

$f_{cc} = \sum_j P_{Tj}^{-12} = 12.13188$

Computing $R: (12)(12.13) \frac{\epsilon^{12}}{R^{13}}$

$\sum_j P_{Dj}^{-6} = 14.45392.$

$-(6)(14.45) \frac{\epsilon^6}{R^7} = 0.$

multiplying by R^7 on each side gives

$(12)(12.13) \frac{\epsilon^{12}}{R^6} - (6)(14.45) \epsilon^6 = 0.$

$(12)(12.13) \epsilon^{12} = (6)(14.45) \epsilon^6 R^6.$

$\left[\frac{(12)(12.13) \epsilon^{12}}{(6)(14.45) \epsilon^6} \right]^{1/6} = R = \left[\frac{(12)(12.13)}{(6)(14.45)} \right]^{1/6} \epsilon$

$\Rightarrow \boxed{R_0/\sigma = 1.09}$. this matches (A) in Kittel.

Thus $R_0 \approx 3.23 \text{ \AA}$.

$\left[(12.13) \left(\frac{\sigma}{R}\right)^{12} - (14.45) \left(\frac{\sigma}{R}\right)^6 \right] \approx 4.3128 - 8.612 \approx -4.2994$

$\epsilon = 50 \times 10^{-16} \text{ erg} = 50 \times 10^{-23} \text{ J} = 5 \times 10^{-22} \text{ J}.$

$U(R) = 2 \times 6.022 \times 10^{23} \times 5 \times 10^{-22} \times (-4.2994) \text{ J/mol}$

$\approx -2.408 \times 10^3 \text{ Joules/mol}$

$\boxed{\approx -2.4 \text{ kJ/mol}}$