

Syllabus for Ch120a Nature of the Chemical Bond

William A. Goddard III

Lecture # Fall 2007 Topic

- 1 10/1 Review QM, role KE in stability of H and bonding in H₂⁺
- 2 10/3 nodal thm, role of KE in bonding of H₂, VB description H₂
- 3 10/5 MO description bonding H₂, symmetry theorem
- 4 10/8 Pauli Princ, spin, Slater det
- 5 10/10 Lack of bonding in He₂, bonding in He₂⁺
- 6 10/12 H atom excited states (1s,2p,3d etc),Li shielding,Aufbau principle
- 7 10/15 MO description Be, B, C,Hund's rule, N, O, F, Ne
- 8 10/17 Bonds to H: FH,OH,NH,BeH,BH,CH
- 9 10/19 CH vs SiH, CF vs CH use VB arguments
- 10 10/22 Symmetry Diatomics, Mulliken correlation Diagram
- 11 10/24 bonding Homonuclear diatomics (Ne₂,F₂,O₂,N₂,N₂⁺,C₂,B₂,Li₂, Li₂⁺)
- 12 10/26 bonding in hydrocarbons (C₂H_x, x=1,2,3; HC bond E)
- 13 10/29 semiconductors: Si,GaAs, GaN. Si(100) surface reconstruction
- 14 10/31 surface reconstruction GaAs(100) 2x4, Si(111) 7x7
- 15 11/2 Hydrocarbons: thermochem, resonance, strain
- 16 11/5 Woodward-Hoffmann Rules cycloaddition, electrocyclic, MO correlation diag
- 17 11/7 Pericyclic reactions, VB view
- 18 11/9 TM Atoms and bonding: reductive elimination, oxidative addition of Pt, Pd compounds
- 19 11/12 MH⁺ diatomics, Exchange, Periodic Trends
- 20 11/14 homogeneous catalysts:metallocene polymerization catalysts
- 21 11/16 homogeneous catalysts: ROMP, Periana CH₄ activation
- 22 11/19 Bulk Metals: Structures, IEM, Binding H,C,O,N to Pt,Ru,Ni surfaces
- 23 11/21 HC reforming/Pt surfaces, fuel cell catalysts
- 24 11/26 Hemoglobin, c-P450
- 25 11/28 Ionic bonding molecules and crystals
- 26 11/30 Hypervalency (XeFn, ClFn, etc), IBX
- 27 12/3 Perovskites (catalyst, supercond., ferroelectric)
- 28 12/5 Fullerenes, bucky tubes, etc
- 29 12/7 superconductors (BCD concept, explain High T_c cuprates)