

Chemical Physics Cumulative Examination
Wednesday, 16 March 2011

One of the important distinctions between the graduate and undergraduate curricula is the seminar program. Graduate students should attend at least one seminar a week while a senior undergraduate might attend one in a semester. A graduate student needs to develop a detailed vocabulary necessary to understand the material presented in seminars.

All of the following terms were used in a Chemistry Department Colloquium given in February by a theoretical physical chemist without explanation. That is, the speaker assumed that the audience understood all of these terms.

Give a concise definition or description of each of the following terms in the context of a chemical physics colloquium. Be sure to label your answers by number.

- 1) AFM tip – Atomic Force Microscope probe
- 2) AO's – Atomic orbitals
- 3) 6-9 potential – Interaction potential with a characteristic shape of $1/r^9 - 1/r^6$
- 4) B3LYP – Becke, three-parameter, Lee-Yang-Parr exchange correlation *functional*
- 5) Band gap – Energy separation between *bands* of states or orbitals in a solid, often a metal
- 6) Band structures – the energy distribution of orbitals in a solid lattice, often a metal
- 7) Bridging ligand – a bidentate (or higher) molecule that spans two different metal atoms
- 8) Carbonyl – generally a C=O function group or a carbon monoxide ligand
- 9) Chemical potential – the change in free energy with number of moles, usually designated by μ
- 10) Complexation – chemical reaction forming a coordination compound or metal ion complex
- 11) Conductance – formally the inverse of the resistance, also a measurement of flow
- 12) Conjugation path – the series of double and single bonds in an (often aromatic) organic molecule
- 13) Continuum states – quantum states in a system that lie above the binding energy
- 14) COO⁻ – acetate functional group (not Chief Operating Officer)
- 15) Cross section – measure of the probability of a reaction with units of Area
- 16) DFT – Density Functional Theory, a quantum modelling theory
- 17) Dihedral angle – formally the angle between two intersecting planes
- 18) EDTA – Ethylene Diamine TetraAcetate, a well-known chelating compound
- 19) Entropy driven reaction – when entropy change is more important than the energy change in a reaction
- 20) Fermi level – highest filled energy level in a set of (closely spaced) energy levels
- 21) Functionalized surface – a macroscopic surface that has had chemical functional group(s) attached
- 22) Geometry optimization – calculational technique to find the molecular structure with lowest energy
- 23) Green's function – a mathematical function used to solve inhomogeneous differential equations
- 24) Ground state – lowest energy state in a quantum mechanical system
- 25) $h\nu$ – literally Planck's constant times frequency, the energy of a photon, sometimes represents a photon

- 26) In-situ synthesis – chemical synthesis or production of a desired produce *in place*
- 27) Labile – easily changed, replaced or chemically substituted
- 28) LUMO/HOMO gap – Energy separation between Lowest Unoccupied and Highest Occupied MO's
- 29) Metal center – generally a metal atom in a biochemical or organic compound
- 30) Molecular degree of freedom – a vibration or rotation of a molecule
- 31) Molecular wire – molecular scale objects that conduct electrical current
- 32) Nonequilibrium population – an *unnatural*, non statistical distribution of the energy in an ensemble
- 33) Orthogonal basis set – a set of mathematical vectors that span a given space
- 34) Overlap integral – the integral over all space of the product of two different wavefunctions
- 35) Peptide – short chain of amino acids, usually much smaller than a protein
- 36) Phonon – generally a collective excitation (vibration) in a solid lattice
- 37) Photocurrent – electrical current induced by photons, i.e., by the photoelectric effect
- 38) π -stacking – stabilization of aromatic compounds by face-to-face interactions of rings
- 39) Potential gradient – the local change in a potential with position, i.e., the local slope
- 40) Pyridine – formally C_5H_5N or a six membered aromatic ring with a nitrogen atom
- 41) QM tunneling – quantum mechanical passage *through* a potential barrier
- 42) Self energy – the calculated total energy of bonds and interactions in a (large) molecule
- 43) Side band of frequency – a higher or lower frequency that results from modulation of two signals
- 44) Spin coupling – the interaction of nuclear angular momenta (spins)
- 45) Square planar complex – four equatorial ligands and no axial ligands in an octahedral compound
- 46) STM – Scanning Tunneling Microscope
- 47) Thermoelectric emission – emission or ejection of electrons solely due to thermal excitation
- 48) Thiol – organic compound with a C-S-H functional group
- 49) Two-state system – a quantum system with only two energy levels (extremely simple system)
- 50) Visible Spectroscopy – energy measurement of photons in the visible region of EM spectrum