

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.

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| 1) AFM tip | 26) In-situ synthesis |
| 2) AO's | 27) Labile |
| 3) 6-9 potential | 28) LUMO/HOMO gap |
| 4) B3LYP | 29) Metal center |
| 5) Band gap | 30) Molecular degree of freedom |
| 6) Band structures | 31) Molecular wire |
| 7) Bridging ligand | 32) Nonequilibrium population |
| 8) Carbonyl | 33) Orthogonal basis set |
| 9) Chemical potential | 34) Overlap integral |
| 10) Complexation | 35) Peptide |
| 11) Conductance | 36) Phonon |
| 12) Conjugation path | 37) Photocurrent |
| 13) Continuum states | 38) π -stacking |
| 14) COO^- | 39) Potential gradient |
| 15) Cross section | 40) Pyridine |
| 16) DFT | 41) QM tunneling |
| 17) Dihedral angle | 42) Self energy |
| 18) EDTA | 43) Side band of frequency |
| 19) Entropy driven reaction | 44) Spin coupling |
| 20) Fermi level | 45) Square planar complex |
| 21) Functionalized surface | 46) STM |
| 22) Geometry optimization | 47) Thermoelectric emission |
| 23) Green's function | 48) Thiol |
| 24) Ground state | 49) Two-state system |
| 25) $h\nu$ | 50) Visible Spectroscopy |