

## Acronyms in Quantum Chemistry (March 2001)

AH Alternating Hydrocarbon  
 AIM Atoms in Molecules, W.Moffitt, Proc.Roy.Soc. (London), **A210**, 245 (1951)  
 AM1 Austin Model 1, newly parametrized MNDO version, M.J.S.Dewar, E.G.Zoebisch, E.F.Healy, J.J.P.Stewart, J.Am.Chem.Soc. **107**, 3902 (1985)  
 AMO Antibonding MO  
 AO Atomic Orbital  
 ASMO Antisymmetrized MO, B3  
 BIGGMOLI ab initio program name  
 BLYP Functional in DFT  
 B3LYP Functional in DFT  
 BMO Bonding MO  
 BO Born-Oppenheimer (-Approximation)  
 BSSE Basis Set Superposition Error, D2  
 CADPAC ab initio program name (CAMbridge Derivative PAcKage)  
 CASSCF Complete Active Space SCF (Version of MCSCF)  
 CC Coupled Cluster, R.J. Bartlett, Ann.Rev.Phys.Chem. **32**, 359 (1981)  
 cc correlation consistent, T. H. Dunning, J.Chem.Phys. **90**, 1007 (1989)  
 CEPA Coupled Electron Pair Approximation, D2, W.Meyer, J.Chem.Phys. **58**,1017 (1973), Int.J.Quantum Chem. **S5**, 341 (1971)  
 CGTF Contracted GTF (=CGTO), D  
 CGTO Contracted GTO (=CGTF), D  
 CHF Coupled Hartree-Fock method, D3, R.M.Stevens, R.M.Pitzer, W.N.Lipscomb, J.Chem.Phys. **38**, 550 (1963), R.Mc Weeney, Phys.Rev.**126**, 1028 (1962)  
 CI Configuration Interaction, A,D  
 CI-SD CI with all Singly and Doubly Excited Configurations, D2,D3  
 CI-SDQ CI-SD with all Quadruply Excited Configurations, D2  
 CNDO Complete Neglect of Differential Overlap, C  
 CNDO/1 CNDO, 1.Version, C, J.A.Pople, D.P.Santry, G.A.Segal, J.Chem.Phys. **43**, S129 (1965), J.A.Pople, G.A.Segal, J.Chem.Phys. **43**, S136 (1965)  
 CNDO/2 CNDO, 2.Version, C, J.A.Pople, G.A.Segal, J.Chem.Phys. **44**, 3289 (1966),  
 CNDO/S CNDO parametrized for spectra (including correlation), J.Del Bene, H.H.Jaffe, J.Chem.Phys. **48**, 1807 (1968)  
 CMO Canonical MO, A  
 CPHF Coupled Perturbed Hartree-Fock, J.Gerratt, I.M.Mills, J.Chem.Phys. **49**, 1719 (1968), Y.Osamura, Y.Yamaguchi, P.Saxe, M.A.Vincent, J.F.Gaw, H.F.Schaefer, Chem.Phys. **72**, 131 (1982)  
 CPMET Coupled Pair MET, D2, J.Cizek, J.Chem.Phys. **45**, 4256 (1966)  
 DE Delocalisation Energy, B  
 DFT Density Functional Theory, G. Parr, W. Yang, "Density-functional theory of atoms and molecules", Clarendon, Oxford 1989  
 DIIS Direct Inversion of the Iterative Subspace (convergence accelerator)  
 DIM Diatomics in Molecules, F.O.Ellison, J.Am.Chem.Soc. **85**, 3540 (1963), J.C.Tully, J.Chem.Phys. **58**,1396 (1973), E.Steiner, P.R.Certain, P.J.Kuntz, J.Chem.Phys. **59**, 47 (1973)  
 DODS Different Orbitals for Different Spins (=UHF), A  
 DZ Double-Zeta Basis Set , A, D  
 DZ+P DZ plus Polarization Basis Set, A, D  
 ECP Effective Core Potential, L.R.Kahn, P.Baybutt, D.G.Truhlar, J.Chem.Phys. **65**, 3826 (1976)  
 ECPMET Extended CPMET, D2, J.Paldus, J.Cizek, I.Shavitt, Phys.Rev. **A5**, 50 (1972)  
 EFV Electric Field Variant (Basis Set), A.J.Sadlej, Chem.Phys.Letters **47**, 50 (1977)  
 EHT Extended Hueckel Theory, A, R.Hoffmann, J.Chem.Phys. **39**, 1397(1963),

S.Z.Engelke, Ch.L.Beckel, Int.J.Quant.Chem. **Symp. 8**, 209 (1974)  
 EMZDO Exchange Modified ZDO, R.N.Dixon, Mol.Phys.**12**, 83 (1967)  
 EPCE Effective Pair Correlation Energy, D2, O.Sinanoglu, H.Oe.Pamuk, Theor.Chim.Acta **27**, 289 (1972)  
 EPCE-F2 EPCE with F2-approximation extended to skeleton, H.O.Pamuk, Theor.Chim.Acta **28**, 85 (1972), O.Sinanoglu, H.O.Pamuk, J.Am.Chem.Soc. **95**, 5435 (1973)  
 EPV Exclusion Principle Violating, D2,  
 FE Frees Electron  
 FIM Fragments-in-Molecules, M.Klessinger, Theor.Chim.Acta **49**, 77 (1978)  
 FOGO Floating Orbital Geometry Optimization, H.Huber, Chem.Phys.Letters **62**, 95 (1979), Theor.Chim.Acta **55**, 117 (1980)  
 FORS Full Optimized Reaction Space, D.F.Feller, M.W.Schmidt, K.J.Ruedenberg, J.Am.Chem.Soc. **104**, 960 (1982)  
 FP-INDO Finite Perturbation INDO, G.E.Maciel,J.W.Mc Iver, N.S.Ostlund, J.A.Pople, J.Am.Chem.Soc. **92**, 1 (1970)  
 FRC Frozen Core, M.Jungen, Theor.Chim.Acta **60**, 369 (1981)  
 FSGO Floating Spherical Gaussian Orbitals, D2, D3, A.A.Frost, J.Chem.Phys. **47**, 3707, 3714 (1967), A.A.Frost, R.A.Rouse, L.Vescelius, nt.J.Quant.Chem. **2S**, 43 (1968)  
 G2 GAUSSIAN-2, L.A.Curtiss, K.Raghavachari, G.W.Trucks, J.A.Pople, J.Chem.Phys. **94**, 7221 (1991)  
 GAUSSIAN ab initio program name  
 GGA Generalized Gradient Approach (DFT approximation)  
 GIAO Gauge Invariant AO, R.Ditchfield, J.Chem.Phys. **56**, 5688 (1972)  
 GTF Gaussian Type Function (=GTO), A, D  
 GTO Gaussian Type Orbital (=GTF), A, D  
 GVB Generalized VB  
 HAM Hydrogenic Atoms in Molecules, L.Asbrink, C.Fridh, E.Lindholm, Chem.Phys.Letters **52**, 63, 69, 72 (1977), **66**, 411(1979)  
 HF Hartree-Fock, A, C, D  
 HFR HF-Roothaan, A, C, D  
 HMO Hueckel Molecular Orbital Method, A, B, E.Hueckel, Z.Physik, **70**, 204 (1931), **72**, 310 (1931), **76**, 628 (1932)  
 HOMO Highest Occupied MO  
 HONDO ab initio program name, D2, M.Dupuis, J.Rys, H.F.King, J.Chem.Phys. **65**, 111 (1976)  
 IBMOL ab initio program name, D2  
 IEPA Independent Electron Pair Approximation, D2, R.Ahrlrichs, H.Lischka, V.Staemmler, W.Kutzelnigg, J.Chem. Phys. **62**, 1225 (1975), M.Jungen, R.Ahrlrichs, Theor.Chim. Acta **17**, 339 (1970)  
 IGLO Individual Gauge for Localized Orbitals, Method for the Calculation of NMR-Shifts, W.Kutzelnigg, U.Fleischer, M.Schindler, in "NMR, Basic Principles and Progress 23", ed. P.Diehl et.al., Springer, Berlin, 1991  
 IMOA Iterative Maximum Overlap Approximation, A, Z.B.Maksic, K.Kovacevic, A.Mogus, Theor.Chim.Acta **55**, 127 (1980)  
 INDO Intermediate Neglect of Differential Overlap, A, C, J.A.Pople, D.L.Beveridge, P.A.Dobosh, J.Chem.Phys. **47**, 2026 (1967)  
 INDO/S INDO parametrized for spectra (including correlation), J.Ridley, M.Zerner, Theor.Chim.Acta **32**, 111 (1973)  
 INO Iterative Natural Orbital Method, D2, C.F.Bender, E.R.Davidson, J.Phys.Chem. **70**, 2675 (1966)  
 IRDO Intermediate Retention of Differential Overlap, C3  
 IVO Improved Virtual Orbitals (s.a. FRC), W.Hunt,W.J.Goddard, Chem.Phys.Letters **3**, 414 (1969)  
 KS Kohn-Sham (-orbitals or theory; -> DFT)  
 LCAO Linear Combination of AO's  
 LCBO Linear Combination of Bond Orbitals, A, G.G.Hall, Proc.Roy.Soc. (London) **A205**,

LCBO	Linear Combination of Bond Orbitals, A, G.G.Hall, Proc.Roy.Soc. (London) <b>A205</b> , 541 (1951)		
LCMO	Linear Combination of MO's, B1,C2, M.J.S.Dewar, Proc.Cambridge Phil.Soc. <b>45</b> , 639 (1949)		
LDA	Local Density Approximation (DFT approximation)		
LEMAOnG	Least Energy Minimal Atomic Orbitals (Basis Set), R.Ditchfield, W.J.Hehre, J.A.Pople, J.Chem.Phys. <b>52</b> , 5001(1970)		
LMO	Localized MO, W.England, L.S.Salmon, K.Ruedenberg, Fortschr.chem.Forschung <b>23</b> , 31 (1971), S.F.Boys, Rev.mod.Phys. <b>32</b> , 296 (1960), W.v.Niessen, J.Chem.Phys. <b>56</b> , 4290 (1972), Theor.Chim.Acta <b>27</b> , 9 (1972)		
LNDO/S	Local Neglect of Differential Overlap (including correlation), G.Lauer, K.W.Schulte, A.Schweig, J.Am.Chem.Soc. <b>100</b> , 4925 (1978)		
LO	Localized Orbital (s.a. LMO), C2		
LSD	Local Spin Density (DFT approximation)		
LSDA	Local Spin Density Approximation (DFT approximation)		
LUMO	Lowest Unoccupied MO		
MAO	Modified AO, R.Heinzmann, R.Ahlrichs, Theor.Chim.Acta <b>42</b> , 33 (1976)		
MB	Minimal Basis, A, D		
MBPT	Many Body Perturbation Theory, D3, J.Goldstone, Proc.Roy.Soc.(London) <b>A239</b> , 267 (1957), H.P.Kelly, Advan.Chem.Phys. <b>14</b> , 129 (1969)		
MB-RSPT	Many Body Raleigh-Schrodinger Perturbation Theory, D2, I.Hubac, P.Carsky, Fortschr.chem.Forschung <b>75</b> , 97 (1978)		
MCSCF	Multi Configuration SCF, D2, D3, D.R.Hartree, W.Hartree, B.Swirls, Phil.Trans.Roy.Soc. (London) <b>A238</b> , 229 (1939)		
MET	Many Electron Theory, D2, O.Sinanoglu, J.Chem.Phys. <b>36</b> , 706 (1962)		
MINDO	Modified INDO (s.a. MINDO/1) A, C2, C3		
MINDO/1	1. Version of MINDO, N.C.Baird, M.J.S.Dewar, J.Chem.Phys. <b>50</b> , 1262 (1969)		
MINDO/2	2. Version of MINDO, M.J.S.Dewar, E.Haselbach, J.Am.Chem.Soc. <b>92</b> , 590 (1970)		
MINDO/3	3. Version of MINDO, R.C.Bingham, M.J.S.Dewar, D.H.Lo, J.Am.Chem.Soc. <b>97</b> , 1285 (1975)		
MIM	Molecules-in-Molecules, W.von Niessen, J.Chem.Phys. <b>55</b> , 1948 (1971)		
MM	Molecular Mechanics; not a quantum chemical method. (Force-Field-Calculations)		
MNDDO	Modified NDDO (s.MNDO)		
MNDO	Modified Neglect of Diatomic Overlaps (New name for MNDDO), A, M.J.S.Dewar, W.Thiel, J.Am.Chem.Soc. <b>99</b> , 4899, 4907 (1977); Extension to d-orbitals: W.Thiel, A.A. Voitynk, J.Phys.Chem. <b>100</b> , 616 (1996)		
MNDOC	MNDO including correlation (as 2. order perturbation), W.Thiel, J.Am.Chem.Soc. <b>103</b> , 1413, 1420, 1425 (1981)		
MO	Molecular Orbital		
MP	Moeller-Plesset (-Störungsrechnung), A, C2, C3, C.Moeller, M.S.Plesset, Phys.Rev. <b>46</b> , 618 (1934)		
MRCI	Multi-Reference CI		
MS X	Multiple Scattering X, (Semiempirical Method), J.C.Slater, The SCF for Molecules and Solids, Vol.4, McGraw Hill, N.Y., 1974, Phys.bibl.Th175, K.H.Johnson, Adv.Quant.Chem. <b>7</b> , 143 (1973)		
NAH	Non-AH		
NBMO	Non-Bonding MO		
NBO	Natural Bond Orbitals, A.E. Reed, L.A. Curtiss, F.Weinhold, Chem.Rev. <b>88</b> , 899 (1988)		
NDDO	Neglect of Diatomic Differential Overlap, A, C		
NO	Natural Orbital, A		
OAO	Orthogonal AO's, A		
OCE	One Center Expansions		
ω-Method	A, B3, C2, G.W.Wheland, D.W.Mann, J.Chem.Phys. <b>17</b> , 264(1949)		
PCILO	Perturbational CI of LO's, A, S.Diner, J.P.Malrieu, F.Jordan, M.Gilbert, Theor.Chim.Acta <b>15</b> , 100 (1969)		
			Theor.Chim.Acta <b>15</b> , 100 (1969)
		PERTCI	CI and second order Brillouin-Wigner PERTurbation, H-L.Hase, G.Lauer, K-W.Schulte, A.Schweig, Theor.Chim.Acta <b>48</b> , 47 (1978)
		PES	Potential Energy Surface
		PHANTOM	ab initio program name D2
		PM3	J.J.P.Stewart, J.Comp.Chem. <b>10</b> , 209, 221 (1989)
		PMO	Perturbational MO Method (perturbation calculation, usually used for a specially simplified version by Dewar), A, C2
		PNDO	Partial Neglect of Differential Overlap, C2, C3, M.J.S.Dewar, G.Klopman, J.Am.Chem.Soc. <b>89</b> , 3089 (1967)
		PNO	Pair NO (=PSNO), A, D2, D3, C.Edmiston, M.Krauss, J.Chem.Phys. <b>45</b> , 1833 (1966), W.Meyer, Int.J.Quant.Chem. <b>S5</b> , 341 (1971)
		POLYATOM	ab initio program name, D2
		POLYCAL	STO-Integral-Program Name, D2, R.M.Stevens, J.Chem.Phys. <b>52</b> , 1397 (1970)
		PPP	Pariser-Parr-Pople Method, A, C2, C3
		PRDDO	Partial Retention of Diatomic Differential Overlap, T.A.Halgren, W.N.Lipscomb, J.Chem.Phys. <b>58</b> , 1569 (1973)
		PSNO	Pseudo NO (=PNO)
		PUHF	Projected UHF, D3, W.A.Goddard, Phys.Rev. <b>182</b> , 48 (1969)
		QCPE	Quantum Chemical Program Exchange
		QM/MM	Quanten Mechanics combined with Molecular Mechanics, M.J. Field, P.A. Bash, M. Karplus, J.Comp.Chem. <b>11</b> , 700 (1990)
		REPE	Resonance Energy per Electron, B.A.Hess, L.J.Schaad, J.Am.Chem.Soc. <b>93</b> , 305 (1971)
		RHF	Restricted HF Method, A, C, D
		SAMO	Simulated ab initio MO, J.E.Eilers, D.R.Whitman, J.Am.Chem.Soc. <b>95</b> , 2067 (1973), B.J.Duke, B.O'Leary, J.Chem.Phys. <b>79</b> , 3424 (1983)
		S.C.E.	Self Consistent Electronegativity (=VESCF)
		SCF	Self Consistent Field, A, C, D
		SEHF	Spin Extended HF, D3, W.A.Goddard, Phys.Rev. <b>182</b> , 48 (1969)
		SD-CI	(=CI-SD)
		SDQ-CI	(=CI-SDQ)
		SINDO	Symmetrically Orthogonalized INDO, P.Coffey, K.Jug, J.Am.Chem.Soc. <b>95</b> , 7575 (1973)
		SINDO1	New Version of SINDO, K.Jug,D.N.Nanda, Theor.Chim.Acta <b>57</b> , 95, 107, 131 (1980)
		SOHF	Spin Optimized HF, D3, U.Kaldor, F.E.Harris, Phys.Rev. <b>183</b> , 1 (1969)
		SPINDO	Spectroscopic Potentials adjusted INDO, L.Asbrink, C.Fridh, E.Lindholm, J.Am.Chem.Soc. <b>94</b> , 5501 (1972)
		SPO	Split-p-Orbital, C2, M.J.S.Dewar, N.L.Hojvat, J.Chem.Phys. <b>34</b> , 1232 (1961), M.J.S.Dewar, N.L.Sabelli, J.Chem. Phys. <b>36</b> , 2310 (1962)
		STO	Slater Type Orbital
		STO-nG	n=2,3,4,5,6 Basis of STO's expanded by n Gaussian functions, A, D2
		SUHF	Spin UHF (=UHF)
		SV	Split Valence (Basis), D2
		SZO	Slater-Zener-Orbitals (=STO)
		TEXAS	ab initio program name
		UHF	Unrestricted HF, A, C, D
		VB	Valence Bond Method, A
		VESCF	Variable Electronegativity SCF, C3, R.D.Brown, M.L.Heffernan, Trans.Farad.Soc. <b>54</b> , 757 (1958)
		WF	Wave function
		X	(= MS X )
		ZDO	Zero Differential Overlap, A, C