

Results found: 342

Sum of the Times Cited: 22,176

Average Citations per Item: 64.84

h-index: 84

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
1. Author(s): WARSHEL, A; LEVITT, M Title: THEORETICAL STUDIES OF ENZYMIC REACTIONS - DIELECTRIC, ELECTROSTATIC AND STERIC STABILIZATION OF CARBONIUM-ION IN REACTION OF LYSOZYME Source: JOURNAL OF MOLECULAR BIOLOGY, 103 (2): 227-249 1976 ISSN: 0022-2836	96	90	95	99	87	1205	37.66
2. Author(s): WARSHEL, A; RUSSELL, ST Title: CALCULATIONS OF ELECTROSTATIC INTERACTIONS IN BIOLOGICAL-SYSTEMS AND IN SOLUTIONS Source: QUARTERLY REVIEWS OF BIOPHYSICS, 17 (3): 283-422 1984 ISSN: 0033-5835	28	38	29	28	12	756	32.87
3. Author(s): WARSHEL, A; KARPLUS, M Title: CALCULATION OF GROUND AND EXCITED-STATE POTENTIAL SURFACES OF CONJUGATED MOLECULES .1. FORMULATION AND PARAMETRIZATION Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 94 (16): 5612-& 1972 ISSN: 0002-7863	13	5	6	6	1	527	14.64
4. Author(s): LIFSON, S; WARSHEL, A Title: CONSISTENT FORCE FIELD FOR CALCULATIONS OF CONFORMATIONS VIBRATIONAL SPECTRA AND ENTHALPIES OF CYCLOALKANE AND N-ALKANE MOLECULES Source: JOURNAL OF CHEMICAL PHYSICS, 49 (11): 5116-& 1968 ISSN: 0021-9606	12	3	6	3	2	489	12.23
5. Author(s): LEVITT, M; WARSHEL, A Title: COMPUTER-SIMULATION OF PROTEIN FOLDING Source: NATURE, 253 (5494): 694-698 1975 ISSN: 0028-0836	12	16	15	11	12	373	11.30
6. Author(s): Kong, J; White, CA; Krylov, AI; et al. Title: Q-chem 2.0: A high-performance ab initio electronic structure program package Source: JOURNAL OF COMPUTATIONAL CHEMISTRY, 21 (16): 1532-1548 DEC 2000 ISSN: 0192-8651	54	69	86	92	34	371	46.38
7. Author(s): WARSHEL, A Title: DYNAMICS OF REACTIONS IN POLAR-SOLVENTS - SEMI-CLASSICAL TRAJECTORY STUDIES OF ELECTRON-TRANSFER AND PROTON-TRANSFER REACTIONS Source: JOURNAL OF PHYSICAL CHEMISTRY, 86 (12): 2218-2224 1982 ISSN: 0022-3654	19	16	19	23	11	366	14.08
8. Author(s): AQVIST, J; WARSHEL, A Title: SIMULATION OF ENZYME-REACTIONS USING VALENCE-BOND FORCE-FIELDS AND OTHER HYBRID QUANTUM-CLASSICAL APPROACHES Source: CHEMICAL REVIEWS, 93 (7): 2523-2544 NOV 1993 ISSN: 0009-2665	35	26	22	29	23	343	22.87

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
9. Author(s): WARSHEL, A; AQVIST, J Title: ELECTROSTATIC ENERGY AND MACROMOLECULAR FUNCTION Source: ANNUAL REVIEW OF BIOPHYSICS AND BIOPHYSICAL CHEMISTRY, 20: 267-298 1991 ISSN: 0084-6589	19	18	19	12	5	340	20.00
10. Author(s): WARSHEL, A; LIFSON, S Title: CONSISTENT FORCE FIELD CALCULATIONS .2. CRYSTAL STRUCTURES, SUBLIMATION ENERGIES, MOLECULAR AND LATTICE VIBRATIONS, MOLECULAR CONFORMATIONS, AND ENTHALPIES OF ALKANES Source: JOURNAL OF CHEMICAL PHYSICS, 53 (2): 582-& 1970 ISSN: 0021-9606	7	3	4	2	1	326	8.58
11. Author(s): WARSHEL, A; NARAYSZABO, G; SUSSMAN, F; et al. Title: HOW DO SERINE PROTEASES REALLY WORK Source: BIOCHEMISTRY, 28 (9): 3629-3637 MAY 2 1989 ISSN: 0006-2960	13	14	14	9	10	304	16.00
12. Author(s): WARSHEL, A; WEISS, RM Title: AN EMPIRICAL VALENCE BOND APPROACH FOR COMPARING REACTIONS IN SOLUTIONS AND IN ENZYMES Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 102 (20): 6218-6226 1980 ISSN: 0002-7863	18	22	18	18	21	300	10.71
13. Author(s): WARSHEL, A Title: CALCULATIONS OF CHEMICAL PROCESSES IN SOLUTIONS Source: JOURNAL OF PHYSICAL CHEMISTRY, 83 (12): 1640-1652 1979 ISSN: 0022-3654	9	6	17	12	4	284	9.79
14. Author(s): WARSHEL, A Title: BICYCLE-PEDAL MODEL FOR 1ST STEP IN VISION PROCESS Source: NATURE, 260 (5553): 679-683 1976 ISSN: 0028-0836	8	11	11	16	20	255	7.97
15. Author(s): WARSHEL, A Title: ENERGETICS OF ENZYME CATALYSIS Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA, 75 (11): 5250-5254 1978 ISSN: 0027-8424	13	10	10	15	7	253	8.43
16. Author(s): Schutz, CN; Warshel, A Title: What axe the dielectric "constants" of proteins and how to validate electrostatic models? Source: PROTEINS-STRUCTURE FUNCTION AND GENETICS, 44 (4): 400-417 SEP 1 2001 ISSN: 0887-3585	41	56	49	48	30	248	35.43
17. Author(s): LEE, FS; CHU, ZT; WARSHEL, A Title: MICROSCOPIC AND SEMIMICROSCOPIC CALCULATIONS OF ELECTROSTATIC ENERGIES IN PROTEINS BY THE POLARIS AND ENZYMIK PROGRAMS Source: JOURNAL OF COMPUTATIONAL CHEMISTRY, 14 (2): 161-185 FEB 1993 ISSN: 0192-8651	17	18	13	20	13	230	15.33
18. Author(s): WARSHEL, A; RUSSELL, ST; CHURG, AK Title: MACROSCOPIC MODELS FOR STUDIES OF ELECTROSTATIC INTERACTIONS IN PROTEINS - LIMITATIONS AND APPLICABILITY Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA-BIOLOGICAL SCIENCES, 81 (15): 4785-4789 1984 ISSN: 0027-8424	8	11	6	8	5	220	9.17
19. Author(s): HWANG, JK; WARSHEL, A Title: MICROSCOPIC EXAMINATION OF FREE-ENERGY RELATIONSHIPS FOR ELECTRON-TRANSFER IN POLAR-SOLVENTS Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 109 (3): 715-720 FEB 4 1987 ISSN: 0002-7863	7	11	9	14	5	215	10.24
20. Author(s): KING, G; WARSHEL, A Title: A SURFACE CONSTRAINED ALL-ATOM SOLVENT MODEL FOR EFFECTIVE SIMULATIONS OF POLAR SOLUTIONS Source: JOURNAL OF CHEMICAL PHYSICS, 91 (6): 3647-3661 SEP 15 1989	15	20	12	26	9	213	11.21

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
ISSN: 0021-9606							
21.	Author(s): LEVITT, M; WARSHEL, A Title: EXTREME CONFORMATIONAL FLEXIBILITY OF FURANOSE RING IN DNA AND RNA Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 100 (9): 2607-2613 1978 ISSN: 0002-7863						7.10
22.	Author(s): WARSHEL, A; KARPLUS, M Title: CALCULATION OF π π EXCITED-STATE CONFORMATIONS AND VIBRONIC STRUCTURE OF RETINAL AND RELATED MOLECULES Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 96 (18): 5677-5689 1974 ISSN: 0002-7863						6.24
23.	Author(s): WARSHEL, A Title: ELECTROSTATIC BASIS OF STRUCTURE-FUNCTION CORRELATION IN PROTEINS Source: ACCOUNTS OF CHEMICAL RESEARCH, 14 (9): 284-290 1981 ISSN: 0001-4842						7.81
24.	Author(s): WARSHEL, A; DAUBER, P Title: CALCULATIONS OF RESONANCE RAMAN-SPECTRA OF CONJUGATED MOLECULES Source: JOURNAL OF CHEMICAL PHYSICS, 66 (12): 5477-5488 1977 ISSN: 0021-9606						6.71
25.	Author(s): HWANG, JK; KING, G; CREIGHTON, S; et al. Title: SIMULATION OF FREE-ENERGY RELATIONSHIPS AND DYNAMICS OF SN2 REACTIONS IN AQUEOUS-SOLUTION Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 110 (16): 5297-5311 AUG 3 1988 ISSN: 0002-7863						10.30
26.	Author(s): WARSHEL, A; PAPAZYAN, A; KOLLMAN, PA Title: ON LOW-BARRIER HYDROGEN-BONDS AND ENZYME CATALYSIS Source: SCIENCE, 269 (5220): 102-104 JUL 7 1995 ISSN: 0036-8075						15.69
27.	Author(s): PARSON, WW; WARSHEL, A Title: SPECTROSCOPIC PROPERTIES OF PHOTOSYNTHETIC REACTION CENTERS .2. APPLICATION OF THE THEORY TO RHODOPSEUDOMONAS-VIRIDIS Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 109 (20): 6152-6163 SEP 30 1987 ISSN: 0002-7863						9.52
28.	Author(s): WARSHEL, A Title: CALCULATION OF VIBRONIC STRUCTURE OF π - π^* TRANSITION OF TRANS-STILBENE AND CIS-STILBENE Source: JOURNAL OF CHEMICAL PHYSICS, 62 (1): 214-221 1975 ISSN: 0021-9606						6.03
29.	Author(s): Warshel, A Title: Electrostatic origin of the catalytic power of enzymes and the role of preorganized active sites Source: JOURNAL OF BIOLOGICAL CHEMISTRY, 273 (42): 27035-27038 OCT 16 1998 ISSN: 0021-9258						19.80
30.	Author(s): RUSSELL, ST; WARSHEL, A Title: CALCULATIONS OF ELECTROSTATIC ENERGIES IN PROTEINS - THE ENERGETICS OF IONIZED GROUPS IN BOVINE PANCREATIC TRYPSIN-INHIBITOR Source: JOURNAL OF MOLECULAR BIOLOGY, 185 (2): 389-404 1985 ISSN: 0022-2836						8.57
31.	Author(s): PARSON, WW; CHU, ZT; WARSHEL, A Title: ELECTROSTATIC CONTROL OF CHARGE SEPARATION IN BACTERIAL PHOTOSYNTHESIS Source: BIOCHIMICA ET BIOPHYSICA ACTA, 1017 (3): 251-272 JUN 26 1990 ISSN: 0006-3002						10.89
32.	Author(s): KING, G; WARSHEL, A Title: INVESTIGATION OF THE FREE-ENERGY FUNCTIONS FOR ELECTRON-TRANSFER REACTIONS						11.41

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
	Source: JOURNAL OF CHEMICAL PHYSICS, 93 (12): 8682-8692 DEC 15 1990 ISSN: 0021-9606						
33.	0	2	1	3	3	190	6.13
	Author(s): WARSHEL, A Title: INTERPRETATION OF RESONANCE RAMAN-SPECTRA OF BIOLOGICAL MOLECULES Source: ANNUAL REVIEW OF BIOPHYSICS AND BIOENGINEERING, 6: 273-300 1977 ISSN: 0084-6589						
34.	8	15	9	13	4	181	6.70
	Author(s): WARSHEL, A Title: CALCULATIONS OF ENZYMIC-REACTIONS - CALCULATIONS OF PKA, PROTON-TRANSFER REACTIONS, AND GENERAL ACID CATALYSIS REACTIONS IN ENZYMES Source: BIOCHEMISTRY, 20 (11): 3167-3177 1981 ISSN: 0006-2960						
35.	13	13	14	21	6	179	11.19
	Author(s): LEE, FS; WARSHEL, A Title: A LOCAL REACTION FIELD METHOD FOR FAST EVALUATION OF LONG-RANGE ELECTROSTATIC INTERACTIONS IN MOLECULAR SIMULATIONS Source: JOURNAL OF CHEMICAL PHYSICS, 97 (5): 3100-3107 SEP 1 1992 ISSN: 0021-9606						
36.	16	13	8	10	6	178	10.47
	Author(s): KING, G; LEE, FS; WARSHEL, A Title: MICROSCOPIC SIMULATIONS OF MACROSCOPIC DIELECTRIC-CONSTANTS OF SOLVATED PROTEINS Source: JOURNAL OF CHEMICAL PHYSICS, 95 (6): 4366-4377 SEP 15 1991 ISSN: 0021-9606						
37.	6	6	5	11	3	178	8.09
	Author(s): CHURG, AK; WARSHEL, A Title: CONTROL OF THE REDOX POTENTIAL OF CYTOCHROME-C AND MICROSCOPIC DIELECTRIC EFFECTS IN PROTEINS Source: BIOCHEMISTRY, 25 (7): 1675-1681 APR 8 1986 ISSN: 0006-2960						
38.	2	0	1	0	2	177	4.66
	Author(s): WARSHEL, A; LEVITT, M; LIFSON, S Title: CONSISTENT FORCE FIELD FOR CALCULATION OF VIBRATIONAL SPECTRA AND CONFORMATIONS OF SOME AMIDES AND LACTAM RINGS Source: JOURNAL OF MOLECULAR SPECTROSCOPY, 33 (1): 84-& 1970 ISSN: 0022-2852						
39.	18	27	15	21	10	175	15.91
	Author(s): Sham, YY; Chu, ZT; Warshel, A Title: Consistent calculations of pK(a)'s of ionizable residues in proteins: Semi-microscopic and microscopic approaches Source: JOURNAL OF PHYSICAL CHEMISTRY B, 101 (22): 4458-4472 MAY 29 1997 ISSN: 1089-5647						
40.	10	7	3	2	0	168	10.50
	Author(s): LUZHKOVA, V; WARSHEL, A Title: MICROSCOPIC MODELS FOR QUANTUM-MECHANICAL CALCULATIONS OF CHEMICAL PROCESSES IN SOLUTIONS - LD/AMPAC AND SCAAS/AMPAC CALCULATIONS OF SOLVATION ENERGIES Source: JOURNAL OF COMPUTATIONAL CHEMISTRY, 13 (2): 199-213 MAR 1992 ISSN: 0192-8651						
41.	16	11	18	14	5	165	13.75
	Author(s): Stephens, PJ; Jollie, DR; Warshel, A Title: Protein control of redox potentials of iron-sulfur proteins Source: CHEMICAL REVIEWS, 96 (7): 2491-2513 NOV 1996 ISSN: 0009-2665						
42.	5	7	3	9	3	165	7.50
	Author(s): WARSHEL, A; HWANG, JK Title: SIMULATION OF THE DYNAMICS OF ELECTRON-TRANSFER REACTIONS IN POLAR-SOLVENTS - SEMICLASSICAL TRAJECTORIES AND DISPERSED POLARON APPROACHES Source: JOURNAL OF CHEMICAL PHYSICS, 84 (9): 4938-4957 MAY 1 1986 ISSN: 0021-9606						

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	1364	1399	1267	1711	1059	22,176	554.40
43. Author(s): WARSHEL, A; CHU, ZT; PARSON, WW Title: DISPERSED POLARON SIMULATIONS OF ELECTRON-TRANSFER IN PHOTOSYNTHETIC REACTION CENTERS Source: SCIENCE, 246 (4926): 112-116 OCT 6 1989 ISSN: 0036-8075	8	6	3	6	5	158	8.32
44. Author(s): Florian, J; Warshel, A Title: Langevin dipoles model for ab initio calculations of chemical processes in solution: Parametrization and application to hydration free energies of neutral and ionic solutes and conformational analysis in aqueous solution Source: JOURNAL OF PHYSICAL CHEMISTRY B, 101 (28): 5583-5595 JUL 10 1997 ISSN: 1089-5647	15	13	24	23	8	157	14.27
45. Author(s): Warshel, A; Papazyan, A Title: Electrostatic effects in macromolecules: fundamental concepts and practical modeling Source: CURRENT OPINION IN STRUCTURAL BIOLOGY, 8 (2): 211-217 APR 1998 ISSN: 0959-440X	19	18	12	12	6	156	15.60
46. Author(s): WARSHEL, A; SUSSMAN, F; KING, G Title: FREE-ENERGY OF CHARGES IN SOLVATED PROTEINS - MICROSCOPIC CALCULATIONS USING A REVERSIBLE CHARGING PROCESS Source: BIOCHEMISTRY, 25 (26): 8368-8372 DEC 30 1986 ISSN: 0006-2960	3	7	7	11	5	148	7.05
47. Author(s): CHURG, AK; WEISS, RM; WARSHEL, A; et al. Title: ON THE ACTION OF CYTOCHROME-C - CORRELATING GEOMETRY CHANGES UPON OXIDATION WITH ACTIVATION-ENERGIES OF ELECTRON-TRANSFER Source: JOURNAL OF PHYSICAL CHEMISTRY, 87 (10): 1683-1694 1983 ISSN: 0022-3654	4	2	3	4	0	146	5.84
48. Author(s): WARSHEL, A; PARSON, WW Title: SPECTROSCOPIC PROPERTIES OF PHOTOSYNTHETIC REACTION CENTERS .1. THEORY Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 109 (20): 6143-6152 SEP 30 1987 ISSN: 0002-7863	7	3	1	5	2	145	6.90
49. Author(s): WARSHEL, A; SUSSMAN, F; HWANG, JK Title: EVALUATION OF CATALYTIC FREE-ENERGIES IN GENETICALLY MODIFIED PROTEINS Source: JOURNAL OF MOLECULAR BIOLOGY, 201 (1): 139-159 MAY 5 1988 ISSN: 0022-2836	5	6	1	6	2	141	7.05
50. Author(s): CREIGHTON, S; HWANG, JK; WARSHEL, A; et al. Title: SIMULATING THE DYNAMICS OF THE PRIMARY CHARGE SEPARATION PROCESS IN BACTERIAL PHOTOSYNTHESIS Source: BIOCHEMISTRY, 27 (2): 774-781 JAN 26 1988 ISSN: 0006-2960	3	5	2	2	0	140	7.00
51. Author(s): SCHWEINS, T; GEYER, M; SCHEFFZEK, K; et al. Title: SUBSTRATE-ASSISTED CATALYSIS AS A MECHANISM FOR GTP HYDROLYSIS OF P21(RAS) AND OTHER GTP-BINDING PROTEINS Source: NATURE STRUCTURAL BIOLOGY, 2 (1): 36-44 JAN 1995 ISSN: 1072-8368	6	15	7	8	2	134	10.31
52. Author(s): LUZHKOVA, V; WARSHEL, A Title: MICROSCOPIC CALCULATIONS OF SOLVENT EFFECTS ON ABSORPTION-SPECTRA OF CONJUGATED MOLECULES Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 113 (12): 4491-4499 JUN 5 1991 ISSN: 0002-7863	4	3	6	6	3	131	7.71
53. Author(s): Villa, J; Warshel, A Title: Energetics and dynamics of enzymatic reactions Source: JOURNAL OF PHYSICAL CHEMISTRY B, 105 (33): 7887-7907 AUG 23 2001 ISSN: 1089-5647	27	32	18	27	12	130	18.57

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	1364	1399	1267	1711	1059	22,176	554.40
54. Author(s): ROWAN, R; WARSHEL, A; SYKES, BD; et al. Title: CONFORMATION OF RETINAL ISOMERS Source: BIOCHEMISTRY, 13 (5): 970-981 1974 ISSN: 0006-2960	0	0	1	0	1	130	3.82
55. Author(s): WARSHEL, A Title: CONVERSION OF LIGHT ENERGY TO ELECTROSTATIC ENERGY IN THE PROTON PUMP OF HALOBACTERIUM-HALOBIIUM Source: PHOTOCHEMISTRY AND PHOTOBIOLOGY, 30 (2): 285-290 1979 ISSN: 0031-8655	5	7	3	5	3	129	4.45
56. Author(s): WARSHEL, A; PARSON, WW Title: COMPUTER-SIMULATIONS OF ELECTRON-TRANSFER REACTIONS IN SOLUTION AND IN PHOTOSYNTHETIC REACTION CENTERS Source: ANNUAL REVIEW OF PHYSICAL CHEMISTRY, 42: 279-309 1991 ISSN: 0066-426X	4	3	4	3	3	128	7.53
57. Author(s): WARSHEL, A; RUSSELL, S Title: THEORETICAL CORRELATION OF STRUCTURE AND ENERGETICS IN THE CATALYTIC REACTION OF TRYPSIN Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 108 (21): 6569-6579 OCT 15 1986 ISSN: 0002-7863	3	8	2	5	2	127	5.77
58. Author(s): WARSHEL, A; BARBOY, N Title: ENERGY-STORAGE AND REACTION PATHWAYS IN THE 1ST STEP OF THE VISION PROCESS Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 104 (6): 1469-1476 1982 ISSN: 0002-7863	7	8	2	4	4	127	4.88
59. Author(s): WARSHEL, A Title: CHARGE STABILIZATION MECHANISM IN VISUAL AND PURPLE MEMBRANE PIGMENTS Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA, 75 (6): 2558-2562 1978 ISSN: 0027-8424	2	2	2	1	2	127	4.23
60. Author(s): AQVIST, J; LUECKE, H; QUIOCHO, FA; et al. Title: DIPOLES LOCALIZED AT HELIX TERMINI OF PROTEINS STABILIZE CHARGES Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA, 88 (5): 2026-2030 MAR 1991 ISSN: 0027-8424	9	7	4	5	1	125	7.35
61. Author(s): LEE, FS; CHU, ZT; BOLGER, MB; et al. Title: CALCULATIONS OF ANTIBODY ANTIGEN INTERACTIONS - MICROSCOPIC AND SEMIMICROSCOPIC EVALUATION OF THE FREE-ENERGIES OF BINDING OF PHOSPHORYLCHOLINE ANALOGS TO MCPC603 Source: PROTEIN ENGINEERING, 5 (3): 215-228 APR 1992 ISSN: 0269-2139	11	9	7	13	7	123	7.69
62. Author(s): Sham, YY; Muegge, I; Warshel, A Title: The effect of protein relaxation on charge-charge interactions and dielectric constants of proteins Source: BIOPHYSICAL JOURNAL, 74 (4): 1744-1753 APR 1998 ISSN: 0006-3495	16	18	11	11	3	120	12.00
63. Author(s): WESOLOWSKI, TA; WARSHEL, A Title: FROZEN DENSITY-FUNCTIONAL APPROACH FOR AB-INITIO CALCULATIONS OF SOLVATED MOLECULES Source: JOURNAL OF PHYSICAL CHEMISTRY, 97 (30): 8050-8053 JUL 29 1993 ISSN: 0022-3654	14	11	16	12	10	119	7.93
64. Author(s): WARSHEL, A Title: ENERGY-STRUCTURE CORRELATION IN METALLOPORPHYRINS AND CONTROL OF OXYGEN BINDING BY HEMOGLOBIN Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA, 74 (5): 1789-1793 1977 ISSN: 0027-8424	0	1	2	2	1	117	3.77

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
65. Author(s): WARSHEL, A; KARPLUS, M Title: VIBRATIONAL STRUCTURE OF ELECTRONIC TRANSITIONS IN CONJUGATED MOLECULES Source: CHEMICAL PHYSICS LETTERS, 17 (1): 7-14 1972 ISSN: 0009-2614	5	4	3	1	2	117	3.34
66. Author(s): LANGEN, R; JENSEN, GM; JACOB, U; et al. Title: PROTEIN CONTROL OF IRON-SULFUR CLUSTER REDOX POTENTIALS Source: JOURNAL OF BIOLOGICAL CHEMISTRY, 267 (36): 25625-25627 DEC 25 1992 ISSN: 0021-9258	6	1	4	6	2	115	7.19
67. Author(s): WARSHEL, A Title: DYNAMICS OF ENZYMIC REACTIONS Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA-BIOLOGICAL SCIENCES, 81 (2): 444-448 1984 ISSN: 0027-8424	7	4	3	6	3	115	4.79
68. Author(s): Muegge, I; Qi, PX; Wand, AJ; et al. Title: The reorganization energy of cytochrome c revisited Source: JOURNAL OF PHYSICAL CHEMISTRY B, 101 (5): 825-836 JAN 30 1997 ISSN: 1089-5647	14	10	13	16	7	113	10.27
69. Author(s): WARSHEL, A; CHU, ZT Title: QUANTUM CORRECTIONS FOR RATE CONSTANTS OF DIABATIC AND ADIABATIC REACTIONS IN SOLUTIONS Source: JOURNAL OF CHEMICAL PHYSICS, 93 (6): 4003-4015 SEP 15 1990 ISSN: 0021-9606	1	6	0	7	1	108	6.00
70. Author(s): Florian, J; Warshel, A Title: Phosphate ester hydrolysis in aqueous solution: Associative versus dissociative mechanisms Source: JOURNAL OF PHYSICAL CHEMISTRY B, 102 (4): 719-734 JAN 22 1998 ISSN: 1089-5647	12	14	16	15	14	106	10.60
71. Author(s): HWANG, JK; CHU, ZT; YADAV, A; et al. Title: SIMULATIONS OF QUANTUM-MECHANICAL CORRECTIONS FOR RATE CONSTANTS OF HYDRIDE-TRANSFER REACTIONS IN ENZYMES AND SOLUTIONS Source: JOURNAL OF PHYSICAL CHEMISTRY, 95 (22): 8445-8448 OCT 31 1991 ISSN: 0022-3654	6	4	3	12	6	106	6.62
72. Author(s): KUWAJIMA, S; WARSHEL, A Title: INCORPORATING ELECTRIC POLARIZABILITIES IN WATER WATER INTERACTION POTENTIALS Source: JOURNAL OF PHYSICAL CHEMISTRY, 94 (1): 460-466 JAN 11 1990 ISSN: 0022-3654	3	3	2	2	1	106	5.89
73. Author(s): Warshel, A; Papazyan, A Title: Energy considerations show that low-barrier hydrogen bonds do not offer a catalytic advantage over ordinary hydrogen bonds Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA, 93 (24): 13665-13670 NOV 26 1996 ISSN: 0027-8424	10	10	3	10	5	105	8.75
74. Author(s): Warshel, A Title: Computer simulations of enzyme catalysis: Methods, progress, and insights Source: ANNUAL REVIEW OF BIOPHYSICS AND BIOMOLECULAR STRUCTURE, 32: 425-443 2003 ISSN: 1056-8700	5	18	23	34	21	101	20.20
75. Author(s): WARSHEL, A Title: ROLE OF THE CHLOROPHYLL DIMER IN BACTERIAL PHOTOSYNTHESIS Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA-PHYSICAL SCIENCES, 77 (6): 3105-3109 1980 ISSN: 0027-8424	1	1	0	2	0	101	3.61

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	1364	1399	1267	1711	1059	22,176	554.40
76. Author(s): WARSHEL, A; LAPPICIRELLA, A Title: CALCULATIONS OF GROUND-EXCITED AND EXCITED-STATE POTENTIAL SURFACES FOR CONJUGATED HETEROATOMIC MOLECULES Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 103 (16): 4664-4673 1981 ISSN: 0002-7863	1	0	1	2	1	98	3.63
77. Author(s): WARSHEL, A; AQVIST, J; CREIGHTON, S Title: ENZYMES WORK BY SOLVATION SUBSTITUTION RATHER THAN BY DESOLVATION Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA, 86 (15): 5820-5824 AUG 1989 ISSN: 0027-8424	5	3	4	6	1	95	5.00
78. Author(s): CUTLER, RL; DAVIES, AM; CREIGHTON, S; et al. Title: ROLE OF ARGININE-38 IN REGULATION OF THE CYTOCHROME-C OXIDATION-REDUCTION EQUILIBRIUM Source: BIOCHEMISTRY, 28 (8): 3188-3197 APR 18 1989 ISSN: 0006-2960	1	4	4	7	0	95	5.00
79. Author(s): AQVIST, J; WARSHEL, A Title: ENERGETICS OF ION PERMEATION THROUGH MEMBRANE CHANNELS - SOLVATION OF NA+ BY GRAMICIDIN-A Source: BIOPHYSICAL JOURNAL, 56 (1): 171-182 JUL 1989 ISSN: 0006-3495	5	2	6	8	0	94	4.95
80. Author(s): JENSEN, GM; WARSHEL, A; STEPHENS, PJ Title: CALCULATION OF THE REDOX POTENTIALS OF IRON-SULFUR PROTEINS - THE 2-/3--COUPLE OF [FE4S4-ASTERISK-CYS(4)] CLUSTERS IN PEPTOCOCCUS-AEROGENES FERREDOXIN, AZOTOBACTER-VINELANDII FERREDOXIN-I, AND CHROMATIUM-VINOSUM HIGH-POTENTIAL IRON PROTEIN Source: BIOCHEMISTRY, 33 (36): 10911-10924 SEP 13 1994 ISSN: 0006-2960	4	1	3	4	0	92	6.57
81. Author(s): WEISS, RM; WARSHEL, A Title: NEW VIEW OF THE DYNAMICS OF SINGLET CIS-TRANS PHOTOISOMERIZATION Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 101 (20): 6131-6133 1979 ISSN: 0002-7863	2	5	5	6	3	88	3.03
82. Author(s): WARSHEL, A; CREIGHTON, S; PARSON, WW Title: ELECTRON-TRANSFER PATHWAYS IN THE PRIMARY EVENT OF BACTERIAL PHOTOSYNTHESIS Source: JOURNAL OF PHYSICAL CHEMISTRY, 92 (9): 2696-2701 MAY 5 1988 ISSN: 0022-3654	0	1	2	1	1	86	4.30
83. Author(s): Hwang, JK; Warshel, A Title: How important are quantum mechanical nuclear motions in enzyme catalysis? Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 118 (47): 11745-11751 NOV 27 1996 ISSN: 0002-7863	8	5	4	12	8	85	7.08
84. Author(s): HONIG, B; WARSHEL, A; KARPLUS, M Title: THEORETICAL STUDIES OF VISUAL CHROMOPHORE Source: ACCOUNTS OF CHEMICAL RESEARCH, 8 (3): 92-100 1975 ISSN: 0001-4842	1	2	0	0	0	85	2.58
85. Author(s): KUAN, TS; WARSHEL, A; SCHNEPP, O Title: INTERMOLECULAR POTENTIALS FOR N2 MOLECULES AND LATTICE VIBRATIONS OF SOLID ALPHA-N2 Source: JOURNAL OF CHEMICAL PHYSICS, 52 (6): 3012-& 1970 ISSN: 0021-9606	0	0	0	0	2	84	2.21
86. Author(s): LANGEN, R; BRAYER, GD; BERGHUIS, AM; et al. Title: EFFECT OF THE ASN52-]ILE MUTATION ON THE REDOX POTENTIAL OF YEAST CYTOCHROME-C - THEORY AND EXPERIMENT Source: JOURNAL OF MOLECULAR BIOLOGY, 224 (3): 589-600 APR 5 1992 ISSN: 0022-2836	5	3	3	2	2	83	5.19

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
87. Author(s): Warshel, A; Parson, WW Title: Dynamics of biochemical and biophysical reactions: insight from computer simulations Source: QUARTERLY REVIEWS OF BIOPHYSICS, 34 (4): 563-679 NOV 2001 ISSN: 0033-5835	20	17	12	14	11	80	13.33
88. Author(s): ALDEN, RG; PARSON, WW; CHU, ZT; et al. Title: CALCULATIONS OF ELECTROSTATIC ENERGIES IN PHOTOSYNTHETIC REACTION CENTERS Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 117 (49): 12284-12298 DEC 13 1995 ISSN: 0002-7863	8	7	5	3	3	80	6.15
89. Author(s): SCHWEINS, T; LANGEN, R; WARSHEL, A Title: WHY HAVE MUTAGENESIS STUDIES NOT LOCATED THE GENERAL BASE IN RAS P21 Source: NATURE STRUCTURAL BIOLOGY, 1 (7): 476-484 JUL 1994 ISSN: 1072-8368	7	4	5	3	3	80	5.71
90. Author(s): WARSHEL, A; CHU, ZT; HWANG, JK Title: THE DYNAMICS OF THE PRIMARY EVENT IN RHODOPSINS REVISITED Source: CHEMICAL PHYSICS, 158 (2-3): 303-314 DEC 15 1991 ISSN: 0301-0104	6	2	3	3	3	79	4.65
91. Author(s): YADAV, A; JACKSON, RM; HOLBROOK, JJ; et al. Title: ROLE OF SOLVENT REORGANIZATION ENERGIES IN THE CATALYTIC ACTIVITY OF ENZYMES Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 113 (13): 4800-4805 JUN 19 1991 ISSN: 0002-7863	5	3	4	4	3	79	4.65
92. Author(s): Warshel, A; Papazyan, A; Muegge, I Title: Microscopic and semimacroscopic redox calculations: What can and cannot be learned from continuum models Source: JOURNAL OF BIOLOGICAL INORGANIC CHEMISTRY, 2 (1): 143-152 FEB 1997 ISSN: 0949-8257	5	7	5	3	2	78	7.09
93. Author(s): MULLER, RP; WARSHEL, A Title: AB-INITIO CALCULATIONS OF FREE-ENERGY BARRIERS FOR CHEMICAL-REACTIONS IN SOLUTION Source: JOURNAL OF PHYSICAL CHEMISTRY, 99 (49): 17516-17524 DEC 7 1995 ISSN: 0022-3654	10	2	5	9	4	78	6.00
94. Author(s): HWANG, JK; WARSHEL, A Title: WHY ION-PAIR REVERSAL BY PROTEIN ENGINEERING IS UNLIKELY TO SUCCEED Source: NATURE, 334 (6179): 270-272 JUL 21 1988 ISSN: 0028-0836	1	3	0	2	0	78	3.90
95. Author(s): WARSHEL, A Title: MICROSCOPIC MODEL FOR CALCULATIONS OF CHEMICAL PROCESSES IN AQUEOUS-SOLUTIONS Source: CHEMICAL PHYSICS LETTERS, 55 (3): 454-458 1978 ISSN: 0009-2614	4	4	3	2	0	76	2.53
96. Author(s): Olsson, MHM; Hong, GY; Warshel, A Title: Frozen density functional free energy simulations of redox proteins: Computational studies of the reduction potential of plastocyanin and rusticyanin Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 125 (17): 5025-5039 APR 30 2003 ISSN: 0002-7863	3	14	23	19	16	75	15.00
97. Author(s): Bentzien, J; Muller, RP; Florian, J; et al. Title: Hybrid ab initio quantum mechanics molecular mechanics calculations of free energy surfaces for enzymatic reactions: The nucleophilic attack in subtilisin Source: JOURNAL OF PHYSICAL CHEMISTRY B, 102 (12): 2293-2301 MAR 19 1998 ISSN: 1089-5647	14	5	4	9	7	75	7.50

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
98. Author(s): Florian, J; Sponer, J; Warshel, A Title: Thermodynamic parameters for stacking and hydrogen bonding of nucleic acid bases in aqueous solution: Ab initio/Langevin dipoles study Source: JOURNAL OF PHYSICAL CHEMISTRY B, 103 (5): 884-892 FEB 4 1999 ISSN: 1089-5647	7	6	6	6	3	74	8.22
99. Author(s): WARSHEL, A Title: MOLECULAR BIOPHYSICS - WHAT ABOUT PROTEIN POLARITY Source: NATURE, 330 (6143): 15-16 NOV 5 1987 ISSN: 0028-0836	2	3	1	2	0	74	3.52
100. Author(s): Villa, J; Strajbl, M; Glennon, TM; et al. Title: How important are entropic contributions to enzyme catalysis? Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA, 97 (22): 11899-11904 OCT 24 2000 ISSN: 0027-8424	17	6	8	12	7	68	8.50
101. Author(s): Sham, YY; Chu, ZT; Tao, H; et al. Title: Examining methods for calculations of binding free energies: LRA, LIE, PDL-D-LRA, and PDL-D/S-LRA calculations of ligands binding to an HIV protease Source: PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS, 39 (4): 393-407 JUN 1 2000 ISSN: 0887-3585	8	15	11	16	7	68	8.50
102. Author(s): HWANG, JK; WARSHEL, A Title: SEMIQUANTITATIVE CALCULATIONS OF CATALYTIC FREE-ENERGIES IN GENETICALLY MODIFIED ENZYMES Source: BIOCHEMISTRY, 26 (10): 2669-2673 MAY 19 1987 ISSN: 0006-2960	3	1	2	1	1	67	3.19
103. Author(s): WARSHEL, A; KARPLUS, M Title: SEMICLASSICAL TRAJECTORY APPROACH TO PHOTOISOMERIZATION Source: CHEMICAL PHYSICS LETTERS, 32 (1): 11-17 1975 ISSN: 0009-2614	1	3	1	1	2	67	2.03
104. Author(s): LANGEN, R; SCHWEINS, T; WARSHEL, A Title: ON THE MECHANISM OF GUANOSINE TRIPHOSPHATE HYDROLYSIS IN RAS P21 PROTEINS Source: BIOCHEMISTRY, 31 (37): 8691-8696 SEP 22 1992 ISSN: 0006-2960	6	5	2	9	3	66	4.12
105. Author(s): Florian, J; Warshel, A Title: A fundamental assumption about OH- attack in phosphate ester hydrolysis is not fully justified Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 119 (23): 5473-5474 JUN 11 1997 ISSN: 0002-7863	6	10	6	7	5	63	5.73
106. Author(s): WARSHEL, A; KING, G Title: POLARIZATION CONSTRAINTS IN MOLECULAR-DYNAMICS SIMULATION OF AQUEOUS-SOLUTIONS - THE SURFACE CONSTRAINT ALL ATOM SOLVENT (SCAAS) MODEL Source: CHEMICAL PHYSICS LETTERS, 121 (1-2): 124-129 1985 ISSN: 0009-2614	3	2	3	9	1	63	2.74
107. Author(s): Warshel, A; Strajbl, M; Villa, J; et al. Title: Remarkable rate enhancement of orotidine 5'-monophosphate decarboxylase is due to transition-state stabilization rather than to ground-state destabilization Source: BIOCHEMISTRY, 39 (48): 14728-14738 DEC 5 2000 ISSN: 0006-2960	8	12	3	9	2	61	7.62
108. Author(s): Strajbl, M; Florian, J; Warshel, A Title: Ab initio evaluation of the potential surface for general base-catalyzed methanolysis of formamide: A reference solution reaction for studies of serine proteases Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 122 (22): 5354-5366 JUN 7 2000 ISSN: 0002-7863	10	11	8	15	5	61	7.62

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
109. Author(s): WESOLOWSKI, T; WARSHEL, A Title: AB-INITIO FREE-ENERGY PERTURBATION CALCULATIONS OF SOLVATION FREE-ENERGY USING THE FROZEN DENSITY-FUNCTIONAL APPROACH Source: JOURNAL OF PHYSICAL CHEMISTRY, 98 (20): 5183-5187 MAY 19 1994 ISSN: 0022-3654	6	5	8	3	2	61	4.36
110. Author(s): Glennon, TM; Villa, J; Warshel, A Title: How does GAP catalyze the GTPase reaction of Ras?: A computer simulation study Source: BIOCHEMISTRY, 39 (32): 9641-9651 AUG 15 2000 ISSN: 0006-2960	9	10	6	12	7	60	7.50
111. Author(s): WARSHEL, A; HULER, E Title: THEORETICAL EVALUATION OF POTENTIAL SURFACES, EQUILIBRIUM GEOMETRIES AND VIBRONIC TRANSITION INTENSITIES OF EXCIMERS - PYRENE CRYSTAL EXCIMER Source: CHEMICAL PHYSICS, 6 (3): 463-468 1974 ISSN: 0301-0104	0	0	0	2	0	60	1.82
112. Author(s): FOTHERGILL, M; GOODMAN, MF; PETRUSKA, J; et al. Title: STRUCTURE-ENERGY ANALYSIS OF THE ROLE OF METAL-IONS IN PHOSPHODIESTER BOND HYDROLYSIS BY DNA-POLYMERASE-I Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 117 (47): 11619-11627 NOV 29 1995 ISSN: 0002-7863	4	4	1	6	3	59	4.54
113. Author(s): AQVIST, J; WARSHEL, A Title: COMPUTER-SIMULATION OF THE INITIAL PROTON-TRANSFER STEP IN HUMAN CARBONIC ANHYDRASE-I Source: JOURNAL OF MOLECULAR BIOLOGY, 224 (1): 7-14 MAR 5 1992 ISSN: 0022-2836	6	2	2	3	5	59	3.69
114. Author(s): WARSHEL, A; SUSSMAN, F Title: TOWARD COMPUTER-AIDED SITE-DIRECTED MUTAGENESIS OF ENZYMES Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA, 83 (11): 3806-3810 JUN 1986 ISSN: 0027-8424	0	1	0	2	0	59	2.68
115. Author(s): WARSHEL, A; WEISS, RM Title: ENERGETICS OF HEME-PROTEIN INTERACTIONS IN HEMOGLOBIN Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 103 (2): 446-451 1981 ISSN: 0002-7863	0	0	1	4	2	59	2.19
116. Author(s): Wesolowski, T; Muller, RP; Warshel, A Title: Ab initio frozen density functional calculations of proton transfer reactions in solution Source: JOURNAL OF PHYSICAL CHEMISTRY, 100 (38): 15444-15449 SEP 19 1996 ISSN: 0022-3654	10	3	4	2	2	58	4.83
117. Author(s): Warshel, A; Florian, J Title: Computer simulations of enzyme catalysis: Finding out what has been optimized by evolution Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA, 95 (11): 5950-5955 MAY 26 1998 ISSN: 0027-8424	11	5	4	5	3	57	5.70
118. Author(s): Schweins, T; Geyer, M; Kalbitzer, HR; et al. Title: Linear free energy relationships in the intrinsic and GTPase activating protein-stimulated guanosine 5'-triphosphate hydrolysis of p21(ras) Source: BIOCHEMISTRY, 35 (45): 14225-14231 NOV 12 1996 ISSN: 0006-2960	5	5	4	4	3	57	4.75
119. Author(s): HWANG, JK; WARSHEL, A Title: A QUANTIZED CLASSICAL PATH APPROACH FOR CALCULATIONS OF QUANTUM-MECHANICAL RATE CONSTANTS Source: JOURNAL OF PHYSICAL CHEMISTRY, 97 (39): 10053-10058 SEP 30 1993 ISSN: 0022-3654	1	5	3	7	2	54	3.60

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
120. Author(s): Warshel, A; Chu, ZT Title: Nature of the surface crossing process in bacteriorhodopsin: Computer simulations of the quantum dynamics of the primary photochemical event Source: JOURNAL OF PHYSICAL CHEMISTRY B, 105 (40): 9857-9871 OCT 11 2001 ISSN: 1089-5647	8	16	8	9	6	53	7.57
121. Author(s): Florian, J; Warshel, A Title: Calculations of hydration entropies of hydrophobic, polar, and ionic solutes in the framework of the Langevin dipoles solvation model Source: JOURNAL OF PHYSICAL CHEMISTRY B, 103 (46): 10282-10288 NOV 18 1999 ISSN: 1089-5647	7	6	3	10	2	53	5.89
122. Author(s): Sham, YY; Muegge, I; Warshel, A Title: Simulating proton translocations in proteins: Probing proton transfer pathways in the Rhodobacter sphaeroides reaction center Source: PROTEINS-STRUCTURE FUNCTION AND GENETICS, 36 (4): 484-500 SEP 1 1999 ISSN: 0887-3585	7	9	5	13	6	52	5.78
123. Author(s): WARSHEL, A; OTTOLENGHI, M Title: KINETIC AND SPECTROSCOPIC EFFECTS OF PROTEIN-CHROMOPHORE ELECTROSTATIC INTERACTIONS IN BACTERIORHODOPSIN Source: PHOTOCHEMISTRY AND PHOTOBIOLOGY, 30 (2): 291-293 1979 ISSN: 0031-8655	0	1	1	1	0	52	1.79
124. Author(s): Shurki, A; Strajbl, M; Villa, J; et al. Title: How much do enzymes really gain by restraining their reacting fragments? Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 124 (15): 4097-4107 APR 17 2002 ISSN: 0002-7863	16	14	6	9	5	51	8.50
125. Author(s): Fuxreiter, M; Warshel, A Title: Origin of the catalytic power of acetylcholinesterase: Computer simulation studies Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 120 (1): 183-194 JAN 14 1998 ISSN: 0002-7863	5	5	5	9	1	51	5.10
126. Author(s): HWANG, JK; CREIGHTON, S; KING, G; et al. Title: EFFECTS OF SOLUTE SOLVENT COUPLING AND SOLVENT SATURATION ON SOLVATION DYNAMICS OF CHARGE-TRANSFER REACTIONS Source: JOURNAL OF CHEMICAL PHYSICS, 89 (2): 859-865 JUL 15 1988 ISSN: 0021-9606	1	3	1	3	0	50	2.50
127. Author(s): Shao, Y; Molnar, LF; Jung, Y; et al. Title: Advances in methods and algorithms in a modern quantum chemistry program package Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 8 (27): 3172-3191 2006 ISSN: 1463-9076				8	41	49	24.50
128. Author(s): Schweins, T; Warshel, A Title: Mechanistic analysis of the observed linear free energy relationships in p21(ras) and related systems Source: BIOCHEMISTRY, 35 (45): 14232-14243 NOV 12 1996 ISSN: 0006-2960	6	6	4	4	2	49	4.08
129. Author(s): AQVIST, J; WARSHEL, A Title: CALCULATIONS OF FREE-ENERGY PROFILES FOR THE STAPHYLOCOCCAL NUCLEASE CATALYZED REACTION Source: BIOCHEMISTRY, 28 (11): 4680-4689 MAY 30 1989 ISSN: 0006-2960	2	0	0	1	0	49	2.58
130. Author(s): WARSHEL, A; LEVITT, M Title: FOLDING AND STABILITY OF HELICAL PROTEINS - CARP MYOGEN Source: JOURNAL OF MOLECULAR BIOLOGY, 106 (2): 421-437 1976 ISSN: 0022-2836	1	1	0	3	2	49	1.53

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
131. Author(s): Shurki, A; Warshel, A Title: Structure/function correlations of proteins using MM, QM/MM, and related approaches: Methods, concepts, pitfalls, and current progress Source: PROTEIN SIMULATIONS ADVANCES IN PROTEIN CHEMISTRY, 66: 249-313 2003 ISSN: 0065-3233	0	4	11	22	11	48	9.60
132. Author(s): Warshel, A Title: Molecular dynamics simulations of biological reactions Source: ACCOUNTS OF CHEMICAL RESEARCH, 35 (6): 385-395 JUN 2002 ISSN: 0001-4842	9	15	14	5	4	48	8.00
133. Author(s): AQVIST, J; WARSHEL, A Title: FREE-ENERGY RELATIONSHIPS IN METALLOENZYME-CATALYZED REACTIONS - CALCULATIONS OF THE EFFECTS OF METAL-ION SUBSTITUTIONS IN STAPHYLOCOCCAL NUCLEASE Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 112 (8): 2860-2868 APR 11 1990 ISSN: 0002-7863	4	1	1	3	4	47	2.61
134. Author(s): PEARSON, JG; OLDFIELD, E; LEE, FS; et al. Title: CHEMICAL-SHIFTS IN PROTEINS - A SHIELDING TRAJECTORY ANALYSIS OF THE FLUORINE NUCLEAR-MAGNETIC-RESONANCE SPECTRUM OF THE ESCHERICHIA-COLI GALACTOSE BINDING-PROTEIN USING A MULTIPOLE SHIELDING POLARIZABILITY LOCAL REACTION FIELD MOLECULAR-DYNAMICS APPROACH Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 115 (15): 6851-6862 JUL 28 1993 ISSN: 0002-7863	2	2	2	2	1	45	3.00
135. Author(s): Burykin, A; Warshel, A Title: What really prevents proton transport through aquaporin? Charge self-energy versus proton wire proposals Source: BIOPHYSICAL JOURNAL, 85 (6): 3696-3706 DEC 2003 ISSN: 0006-3495	1	9	14	13	7	44	8.80
136. Author(s): Florian, J; Strajbl, M; Warshel, A Title: Conformational flexibility of phosphate, phosphonate, and phosphorothioate methyl esters in aqueous solution Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 120 (31): 7959-7966 AUG 12 1998 ISSN: 0002-7863	3	6	5	6	3	44	4.40
137. Author(s): Burykin, A; Schutz, CN; Villa, J; et al. Title: Simulations of ion current in realistic models of ion channels: The KcsA potassium channel Source: PROTEINS-STRUCTURE FUNCTION AND GENETICS, 47 (3): 265-280 MAY 15 2002 ISSN: 0887-3585	11	9	12	6	3	43	7.17
138. Author(s): Strajbl, M; Shurki, A; Kato, M; et al. Title: Apparent NAC effect in chorismate mutase reflects electrostatic transition state stabilization Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 125 (34): 10228-10237 AUG 27 2003 ISSN: 0002-7863	3	10	7	12	9	41	8.20
139. Author(s): Florian, J; Aqvist, J; Warshel, A Title: On the reactivity of phosphate monoester dianions in aqueous solution: Bronsted linear free-energy relationships do not have a unique mechanistic interpretation Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 120 (44): 11524-11525 NOV 11 1998 ISSN: 0002-7863	2	3	6	6	7	41	4.10
140. Author(s): Muegge, I; Schweins, T; Warshel, A Title: Electrostatic contributions to protein-protein binding affinities: Application to Rap/Raf interaction Source: PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS, 30 (4): 407-423 MAR 1 1998 ISSN: 0887-3585	6	10	2	4	2	41	4.10

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
141. Author(s): AQVIST, J; FOTHERGILL, M; WARSHEL, A Title: COMPUTER-SIMULATION OF THE CO2/HCO3- INTERCONVERSION STEP IN HUMAN CARBONIC ANHYDRASE-I Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 115 (2): 631-635 JAN 27 1993 ISSN: 0002-7863	1	2	0	0	1	41	2.73
142. Author(s): Muegge, I; Schweins, T; Langen, R; et al. Title: Electrostatic control of GTP and GDP binding in the oncoprotein p21(ras) Source: STRUCTURE, 4 (4): 475-489 APR 15 1996 ISSN: 0969-2126	3	3	1	4	0	40	3.33
143. Author(s): WARSHEL, A Title: ORIGIN OF THE RED SHIFT OF THE ABSORPTION-SPECTRA OF AGGREGATED CHLOROPHYLLS Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 101 (3): 744-746 1979 ISSN: 0002-7863	0	0	0	0	0	40	1.38
144. Author(s): Aqvist, J; Kolmodin, K; Florian, J; et al. Title: Mechanistic alternatives phosphate monoester hydrolysis: what conclusions can be drawn from available experimental data? Source: CHEMISTRY & BIOLOGY, 6 (3): R71-R80 MAR 1999 ISSN: 1074-5521	6	12	1	4	3	39	4.33
145. Author(s): VAIDEHI, N; WESOLOWSKI, TA; WARSHEL, A Title: QUANTUM-MECHANICAL CALCULATIONS OF SOLVATION FREE-ENERGIES - A COMBINED ABINITIO PSEUDOPOTENTIAL FREE-ENERGY PERTURBATION APPROACH Source: JOURNAL OF CHEMICAL PHYSICS, 97 (6): 4264-4271 SEP 15 1992 ISSN: 0021-9606	5	2	2	3	3	39	2.44
146. Author(s): WARSHEL, A; SCHLOSSER, DW Title: ELECTROSTATIC CONTROL OF THE EFFICIENCY OF LIGHT-INDUCED ELECTRON-TRANSFER ACROSS MEMBRANES Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA-BIOLOGICAL SCIENCES, 78 (9): 5564-5568 1981 ISSN: 0027-8424	2	1	2	1	1	39	1.44
147. Author(s): Alden, RG; Parson, WW; Chu, ZT; et al. Title: Orientation of the OH dipole of tyrosine (M)210 and its effect on electrostatic energies in photosynthetic bacterial reaction centers Source: JOURNAL OF PHYSICAL CHEMISTRY, 100 (41): 16761-16770 OCT 10 1996 ISSN: 0022-3654	8	2	1	2	0	38	3.17
148. Author(s): Florian, J; Goodman, MF; Warshel, A Title: Computer simulation of the chemical catalysis of DNA polymerases: Discriminating between alternative nucleotide insertion mechanisms for T7 DNA polymerase Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 125 (27): 8163-8177 JUL 9 2003 ISSN: 0002-7863	2	9	6	8	11	36	7.20
149. Author(s): WARSHEL, A; CHU, ZT; PARSON, WW Title: ON THE ENERGETICS OF THE PRIMARY ELECTRON-TRANSFER PROCESS IN BACTERIAL REACTION CENTERS Source: JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY, 82 (1-3): 123-128 AUG 23 1994 ISSN: 1010-6030	3	0	3	0	0	36	2.57
150. Author(s): HULER, E; WARSHEL, A Title: INCORPORATION OF INTERMOLECULAR AND INTRAMOLECULAR FORCES IN CALCULATION OF CRYSTAL PACKING AND LATTICE-VIBRATIONS Source: ACTA CRYSTALLOGRAPHICA SECTION B-STRUCTURAL SCIENCE, B 30 (JUL15): 1822-1826 1974 ISSN: 0108-7681	0	0	0	0	0	36	1.06
151. Author(s): Olsson, MHM; Siegbahn, PEM; Warshel, A Title: Simulations of the large kinetic isotope effect and the temperature dependence of the hydrogen atom transfer in lipoxxygenase Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 126 (9): 2820-2828 MAR 10 2004		2	5	19	9	35	8.75

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
ISSN: 0002-7863							
152.	8	6	4	1	4	35	3.50
Author(s): Parson, WW; Chu, ZT; Warshel, A							
Title: Reorganization energy of the initial electron-transfer step in photosynthetic bacterial reaction centers							
Source: BIOPHYSICAL JOURNAL, 74 (1): 182-191 JAN 1998							
ISSN: 0006-3495							
153.	3	1	2	5	2	33	2.20
Author(s): WARSHEL, A; HWANG, JK; AQVIST, J							
Title: COMPUTER-SIMULATIONS OF ENZYMATIC-REACTIONS - EXAMINATION OF LINEAR FREE-ENERGY RELATIONSHIPS AND QUANTUM-MECHANICAL CORRECTIONS IN THE INITIAL PROTON-TRANSFER STEP OF CARBONIC-ANHYDRASE							
Source: FARADAY DISCUSSIONS, 93: 225-238 1992							
ISSN: 0301-7249							
154.	2	3	1	0	1	33	1.50
Author(s): WARSHEL, A							
Title: CORRELATION BETWEEN THE STRUCTURE AND EFFICIENCY OF LIGHT-INDUCED PROTON PUMPS							
Source: METHODS IN ENZYMOLOGY, 127: 578-587 1986							
ISSN: 0076-6879							
155.	4	3	3	5	3	31	3.88
Author(s): Strajbl, M; Sham, YY; Villa, J; et al.							
Title: Calculations of activation entropies of chemical reactions in solution							
Source: JOURNAL OF PHYSICAL CHEMISTRY B, 104 (18): 4578-4584 MAY 11 2000							
ISSN: 1089-5647							
156.	4	4	4	2	1	31	3.10
Author(s): Papazyan, A; Warshel, A							
Title: Continuum and dipole-lattice models of solvation							
Source: JOURNAL OF PHYSICAL CHEMISTRY B, 101 (51): 11254-11264 DEC 18 1997							
ISSN: 1089-5647							
157.	0	0	0	0	1	31	1.03
Author(s): COHEN, MD; HABERKORN, R; HULER, E; et al.							
Title: PAIR-STATES IN ALPHA-PERYLENE CRYSTAL - THEORETICAL-STUDY							
Source: CHEMICAL PHYSICS, 27 (2): 211-216 1978							
ISSN: 0301-0104							
158.	5	5	5	9	5	30	5.00
Author(s): Florian, J; Goodman, MF; Warshel, A							
Title: Theoretical investigation of the binding free energies and key substrate-recognition components of the replication fidelity of human DNA polymerase beta							
Source: JOURNAL OF PHYSICAL CHEMISTRY B, 106 (22): 5739-5753 JUN 6 2002							
ISSN: 1520-6106							
159.	5	2	3	3	4	30	3.00
Author(s): Jensen, GM; Bunte, SW; Warshel, A; et al.							
Title: Energetics of cation radical formation at the proximal active site tryptophan of cytochrome c peroxidase and ascorbate peroxidase							
Source: JOURNAL OF PHYSICAL CHEMISTRY B, 102 (42): 8221-8228 OCT 15 1998							
ISSN: 1089-5647							
160.	2	6	11	8	2	29	5.80
Author(s): Burykin, A; Kato, M; Warshel, A							
Title: Exploring the origin of the ion selectivity of the KcsA potassium channel							
Source: PROTEINS-STRUCTURE FUNCTION AND GENETICS, 52 (3): 412-426 AUG 15 2003							
ISSN: 0887-3585							
161.	6	1	2	4	1	29	2.90
Author(s): Glennon, TM; Warshel, A							
Title: Energetics of the catalytic reaction of ribonuclease A: A computational study of alternative mechanisms							
Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 120 (39): 10234-10247 OCT 7 1998							
ISSN: 0002-7863							
162.	6	4	1	4	2	28	3.50
Author(s): Varnai, P; Warshel, A							
Title: Computer simulation studies of the catalytic mechanism of human aldose reductase							
Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 122 (16): 3849-3860 APR 26 2000							
ISSN: 0002-7863							

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
163. Author(s): Sham, YY; Warshel, A Title: The surface constraint all atom model provides size independent results in calculations of hydration free energies Source: JOURNAL OF CHEMICAL PHYSICS, 109 (18): 7940-7944 NOV 8 1998 ISSN: 0021-9606	5	1	2	8	4	28	2.80
164. Author(s): KONG, YS; WARSHEL, A Title: LINEAR FREE-ENERGY RELATIONSHIPS WITH QUANTUM-MECHANICAL CORRECTIONS - CLASSICAL AND QUANTUM-MECHANICAL RATE CONSTANTS FOR HYDRIDE TRANSFER BETWEEN NAD(+) ANALOGS IN SOLUTIONS Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 117 (23): 6234-6242 JUN 14 1995 ISSN: 0002-7863	1	5	1	3	0	27	2.08
165. Author(s): WARSHEL, A Title: QCFF-PI+MCA PROGRAM PACKAGE EFFICIENCY AND VERSATILITY IN MOLECULAR MECHANICS Source: COMPUTERS & CHEMISTRY, 1 (3): 195-202 1977 ISSN: 0097-8485	2	0	0	0	0	27	0.87
166. Author(s): STILLINGER, FH; HASTED, JB; WARSHEL, A Title: THEORETICAL APPROACHES TO INTERMOLECULAR NATURE OF WATER Source: PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY OF LONDON SERIES B-BIOLOGICAL SCIENCES, 278 (959): 97-112 1977 ISSN: 0962-8436	0	1	0	0	0	27	0.87
167. Author(s): KUWAJIMA, S; WARSHEL, A Title: THE EXTENDED EWALD METHOD - A GENERAL TREATMENT OF LONG-RANGE ELECTROSTATIC INTERACTIONS IN MICROSCOPIC SIMULATIONS Source: JOURNAL OF CHEMICAL PHYSICS, 89 (6): 3751-3759 SEP 15 1988 ISSN: 0021-9606	2	1	2	3	0	26	1.30
168. Author(s): WARSHEL, A; DEAKYNE, C Title: COUPLING OF CHARGE STABILIZATION, TORSION AND BOND ALTERNATION IN LIGHT-INDUCED REACTIONS OF VISUAL PIGMENTS Source: CHEMICAL PHYSICS LETTERS, 55 (3): 459-465 1978 ISSN: 0009-2614	0	1	0	0	0	26	0.87
169. Author(s): Florian, J; Goodman, MF; Warshel, A Title: Free-energy perturbation calculations of DNA destabilization by base substitutions: The effect of neutral guanine thymine, adenine cytosine and adenine difluorotoluene mismatches Source: JOURNAL OF PHYSICAL CHEMISTRY B, 104 (43): 10092-10099 NOV 2 2000 ISSN: 1089-5647	5	2	2	8	1	25	3.12
170. Author(s): WARSHEL, A; SHAKKED, Z Title: THEORETICAL-STUDY OF EXCIMERS IN CRYSTALS OF FLEXIBLE CONJUGATED MOLECULES - EXCIMER FORMATION AND PHOTODIMERIZATION IN CRYSTALLINE 1,4-DIPHENYLBUTADIENE Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 97 (20): 5679-5684 1975 ISSN: 0002-7863	0	0	0	1	1	24	0.73
171. Author(s): HUDSON, B; WARSHEL, A; GORDON, RG Title: MOLECULAR INELASTIC NEUTRON-SCATTERING - COMPUTATIONAL METHODS USING CONSISTENT FORCE-FIELDS Source: JOURNAL OF CHEMICAL PHYSICS, 61 (7): 2929-2939 1974 ISSN: 0021-9606	0	0	1	0	0	24	0.71
172. Author(s): Burykin, A; Warshel, A Title: On the origin of the electrostatic barrier for proton transport in aquaporin Source: FEBS LETTERS, 570 (1-3): 41-46 JUL 16 2004 ISSN: 0014-5793		1	9	7	6	23	5.75
173. Author(s): Warshel, A; Florian, J; Strajbl, M; et al. Title: Circe effect versus enzyme preorganization: What can be learned from the structure of the most proficient enzyme? Source: CHEMBIOCHEM, 2 (2): 109-111 FEB 2 2001 ISSN: 1439-4227	3	5	2	3	0	23	3.29

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
174. Author(s): WARSHEL, A Title: MOLECULAR ORIGIN OF ANOMALOUS POLARIZATION IN RESONANCE RAMAN OF METALLOPORPHYRINS Source: CHEMICAL PHYSICS LETTERS, 43 (2): 273-278 1976 ISSN: 0009-2614	0	0	0	2	1	23	0.72
175. Author(s): Warshel, A; Sharma, PK; Kato, M; et al. Title: Electrostatic basis for enzyme catalysis Source: CHEMICAL REVIEWS, 106 (8): 3210-3235 AUG 9 2006 ISSN: 0009-2665				3	19	22	11.00
176. Author(s): Schutz, CN; Warshel, A Title: Analyzing free energy relationships for proton translocations in enzymes: Carbonic anhydrase revisited Source: JOURNAL OF PHYSICAL CHEMISTRY B, 108 (6): 2066-2075 FEB 12 2004 ISSN: 1520-6106		2	3	9	8	22	5.50
177. Author(s): Strajbl, M; Florian, J; Warshel, A Title: Ab initio evaluation of the free energy surfaces for the general base/acid catalyzed thiolysis of formamide and the hydrolysis of methyl thioformate: A reference solution reaction for studies of cysteine proteases Source: JOURNAL OF PHYSICAL CHEMISTRY B, 105 (19): 4471-4484 MAY 17 2001 ISSN: 1089-5647	5	3	3	6	2	22	3.14
178. Author(s): Schutz, CN; Warshel, A Title: The low barrier hydrogen bond (LBHB) proposal revisited: The case of the asp... his pair in serine proteases Source: PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS, 55 (3): 711-723 MAY 15 2004 ISSN: 0887-3585		1	6	9	5	21	5.25
179. Author(s): Shurki, A; Warshel, A Title: Why does the Ras switch "break" by oncogenic mutations? Source: PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS, 55 (1): 1-10 APR 1 2004 ISSN: 0887-3585		2	7	9	3	21	5.25
180. Author(s): Muegge, I; Tao, H; Warshel, A Title: A fast estimate of electrostatic group contributions to the free energy of protein-inhibitor binding Source: PROTEIN ENGINEERING, 10 (12): 1363-1372 DEC 1997 ISSN: 0269-2139	1	2	1	4	0	21	2.10
181. Author(s): WARSHEL, A; HULER, E; RABINOV, D; et al. Title: EXAMINATION OF INTRAMOLECULAR POTENTIAL SURFACES OF FLEXIBLE CONJUGATED MOLECULES BY CALCULATION OF CRYSTAL-STRUCTURES - EQUILIBRIUM GEOMETRIES OF CHALCONES AND DIPHENYLOCTATETRAENE IN CRYSTAL AND GASEOUS STATE Source: JOURNAL OF MOLECULAR STRUCTURE, 23 (2): 175-191 1974 ISSN: 0022-2860	0	0	0	1	0	21	0.62
182. Author(s): Olsson, MHM; Sharma, PK; Warshel, A Title: Simulating redox coupled proton transfer in cytochrome c oxidase: Looking for the proton bottleneck Source: FEBS LETTERS, 579 (10): 2026-2034 APR 11 2005 ISSN: 0014-5793			2	13	5	20	6.67
183. Author(s): Olsson, MHM; Warshel, A Title: Solute solvent dynamics and energetics in enzyme catalysis: The S(N)2 reaction of dehalogenase as a general benchmark Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 126 (46): 15167-15179 NOV 24 2004 ISSN: 0002-7863		0	5	10	5	20	5.00
184. Author(s): Braun-Sand, S; Strajbl, M; Warshel, A Title: Studies of proton translocations in biological systems: Simulating proton transport in carbonic anhydrase by EVB-based models Source: BIOPHYSICAL JOURNAL, 87 (4): 2221-2239 OCT 2004 ISSN: 0006-3495		0	4	8	8	20	5.00
185. Author(s): Hong, GY; Strajbl, M; Wesolowski, TA; et al. Title: Constraining the electron densities in DFT method as an effective way for ab initio studies of metal-catalyzed reactions Source: JOURNAL OF COMPUTATIONAL CHEMISTRY, 21 (16):	6	2	4	3	1	20	2.50

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
1554-1561 DEC 2000 ISSN: 0192-8651							
186. Author(s): Jenkins, LA; Bashkin, JK; Pennock, JD; et al. Title: Catalytic hydrolysis of adenosine 2',3'-cyclic monophosphate by Cu-II terpyridine Source: INORGANIC CHEMISTRY, 38 (13): 3215-3222 JUN 28 1999 ISSN: 0020-1669	2	3	5	3	0	20	2.22
187. Author(s): Papazyan, A; Warshel, A Title: A stringent test of the cavity concept in continuum dielectrics Source: JOURNAL OF CHEMICAL PHYSICS, 107 (19): 7975-7978 NOV 15 1997 ISSN: 0021-9606	1	2	2	0	1	20	1.82
188. Author(s): WARSHEL, A Title: QUANTUM-MECHANICAL CONSISTENT FORCE-FIELD (QCFF/PI) METHOD - CALCULATIONS OF ENERGIES, CONFORMATIONS AND VIBRONIC INTERACTIONS OF GROUND AND EXCITED-STATES OF CONJUGATED MOLECULES Source: ISRAEL JOURNAL OF CHEMISTRY, 11 (5): 709-717 1973 ISSN: 0021-2148	1	0	0	0	0	20	0.59
189. Author(s): Olsson, MHM; Parson, WW; Warshel, A Title: Dynamical contributions to enzyme catalysis: Critical tests of a popular hypothesis Source: CHEMICAL REVIEWS, 106 (5): 1737-1756 MAY 2006 ISSN: 0009-2665				5	14	19	9.50
190. Author(s): Klahn, M; Braun-Sand, S; Rosta, E; et al. Title: On possible pitfalls in ab initio quantum mechanics/molecular mechanics minimization approaches for studies of enzymatic reactions Source: JOURNAL OF PHYSICAL CHEMISTRY B, 109 (32): 15645-15650 AUG 18 2005 ISSN: 1520-6106			0	10	9	19	6.33
191. Author(s): Strajbl, M; Shurki, A; Warshel, A Title: Converting conformational changes to electrostatic energy in molecular motors: The energetics of ATP synthase Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA, 100 (25): 14834-14839 DEC 9 2003 ISSN: 0027-8424	0	6	3	9	1	19	3.80
192. Author(s): WARSHEL, A; SCHWEINS, T; FOTHERGILL, M Title: LINEAR FREE-ENERGY RELATIONSHIPS IN ENZYMES - THEORETICAL-ANALYSIS OF THE REACTION OF TYROSYL-TRANSFER-RNA SYNTHETASE Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 116 (19): 8437-8442 SEP 21 1994 ISSN: 0002-7863	3	2	1	2	1	19	1.36
193. Author(s): Fuxreiter, M; Warshel, A; Osman, R Title: Role of active site residues in the glycosylase step of T4 Endonuclease V. Computer simulation studies on ionization states Source: BIOCHEMISTRY, 38 (30): 9577-9589 JUL 27 1999 ISSN: 0006-2960	1	1	0	5	0	18	2.00
194. Author(s): WARSHEL, A; STERN, PS; MUKAMEL, S Title: SEMICLASSICAL CALCULATION OF ELECTRONIC-SPECTRA OF SUPERCOOLED ANHARMONIC MOLECULES Source: JOURNAL OF CHEMICAL PHYSICS, 78 (12): 7498-7500 1983 ISSN: 0021-9606	1	0	0	0	0	18	0.72
195. Author(s): WARSHEL, A Title: OXIDATION OF 4A,4B-DIHYDROPHENANTHRENES .3. A THEORETICAL STUDY OF LARGE KINETIC ISOTOPE EFFECT OF DEUTERIUM IN INITIATION STEP OF THERMAL REACTION WITH OXYGEN Source: JOURNAL OF CHEMICAL PHYSICS, 52 (3): 1262-& 1970 ISSN: 0021-9606	0	2	0	2	1	18	0.47
196. Author(s): Florian, J; Goodman, MF; Warshel, A Title: Computer simulations of protein functions: Searching for the molecular origin of the replication fidelity of DNA polymerases Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA, 102 (19): 6819-6824 MAY 10 2005			1	11	5	17	5.67

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
ISSN: 0027-8424							
197.			0	10	6	16	5.33
Author(s): Sharma, PK; Xiang, Y; Kato, M; et al. Title: What are the roles of substrate-assisted catalysis and proximity effects in peptide bond formation by the ribosome? Source: BIOCHEMISTRY, 44 (34): 11307-11314 AUG 30 2005 ISSN: 0006-2960							
198.			1	10	5	16	5.33
Author(s): Braun-Sand, S; Burykin, A; Chu, ZT; et al. Title: Realistic simulations of proton transport along the gramicidin channel: Demonstrating the importance of solvation effects Source: JOURNAL OF PHYSICAL CHEMISTRY B, 109 (1): 583-592 JAN 13 2005 ISSN: 1520-6106							
199.	1	6	3	4	2	16	3.20
Author(s): Barbany, M; Gutierrez-de-Teran, H; Sanz, F; et al. Title: On the generation of catalytic antibodies by transition state analogues Source: CHEMBIOCHEM, 4 (4): 277-285 APR 4 2003 ISSN: 1439-4227							
200.	0	0	0	0	1	16	0.50
Author(s): LIANG, R; SCHNEPP, O; WARSHEL, A Title: RESONANCE RAMAN-SPECTRUM OF AZULENE Source: CHEMICAL PHYSICS LETTERS, 44 (2): 394-398 1976 ISSN: 0009-2614							
201.	0	2	1	4	3	15	1.67
Author(s): Fan, ZZ; Hwang, JK; Warshel, A Title: Using simplified protein representation as a reference potential for all-atom calculations of folding free energy Source: THEORETICAL CHEMISTRY ACCOUNTS, 103 (1): 77-80 NOV 1999 ISSN: 1432-881X							
202.	1	0	0	0	0	15	0.65
Author(s): WARSHEL, A; HWANG, JK Title: QUANTIZED SEMICLASSICAL TRAJECTORY APPROACH FOR EVALUATION OF VIBRONIC TRANSITIONS IN ANHARMONIC MOLECULES Source: JOURNAL OF CHEMICAL PHYSICS, 82 (4): 1756-1771 1985 ISSN: 0021-9606							
203.	3	2	2	6	1	14	2.80
Author(s): Florian, J; Goodman, MF; Warshel, A Title: Computer simulation studies of the fidelity of DNA polymerases Source: BIOPOLYMERS, 68 (3): 286-299 MAR 2003 ISSN: 0006-3525							
204.	1	1	0	1	1	14	1.27
Author(s): Hwang, JK; Warshel, A Title: On the relationship between the dispersed polaron and spin-boson models Source: CHEMICAL PHYSICS LETTERS, 271 (4-6): 223-225 JUN 13 1997 ISSN: 0009-2614							
205.	0	0	1	0	0	14	1.00
Author(s): WARSHEL, A; TAO, H; FOTHERGILL, M; et al. Title: EFFECTIVE METHODS FOR ESTIMATION OF BINDING-ENERGIES IN COMPUTER-AIDED DRUG DESIGN Source: ISRAEL JOURNAL OF CHEMISTRY, 34 (2): 253-256 1994 ISSN: 0021-2148							
206.	1	1	0	1	0	14	0.54
Author(s): WARSHEL, A Title: ENERGETICS OF LIGHT-INDUCED CHARGE SEPARATION ACROSS MEMBRANES Source: ISRAEL JOURNAL OF CHEMISTRY, 21 (4): 341-347 1981 ISSN: 0021-2148							
207.	4	1	1	0	0	13	1.30
Author(s): Parson, WW; Chu, ZT; Warshel, A Title: Oscillations of the energy gap for the initial electron-transfer step in bacterial reaction centers Source: PHOTOSYNTHESIS RESEARCH, 55 (2-3): 147-152 MAR 1998 ISSN: 0166-8595							
208.	0	0	0	0	0	13	0.35
Author(s): WARSHEL, A Title: CALCULATION OF ANHARMONICITY IN VIBRATIONAL FREQUENCIES OF ALKANE MOLECULES BY CFF FUNCTIONS Source: JOURNAL OF CHEMICAL PHYSICS, 55 (7): 3327-& 1971 ISSN: 0021-9606							

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
209. Author(s): Olsson, MHM; Mavri, J; Warshel, A Title: Transition state theory can be used in studies of enzyme catalysis: lessons from simulations of tunnelling and dynamical effects in lipoxxygenase and other systems Source: PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY B-BIOLOGICAL SCIENCES, 361 (1472): 1417-1432 AUG 29 2006 ISSN: 0962-8436				1	11	12	6.00
210. Author(s): Rosta, E; Klahn, M; Warshel, A Title: Towards accurate ab initio QM/MM calculations of free-energy profiles of enzymatic reactions Source: JOURNAL OF PHYSICAL CHEMISTRY B, 110 (6): 2934-2941 FEB 16 2006 ISSN: 1520-6106				4	8	12	6.00
211. Author(s): Parson, WW; Warshel, A Title: A density-matrix model of photosynthetic electron transfer with microscopically estimated vibrational relaxation times Source: CHEMICAL PHYSICS, 296 (2-3): 201-216 JAN 26 2004 ISSN: 0301-0104		2	4	5	1	12	3.00
212. Author(s): Florian, J; Warshel, A; Goodman, MF Title: Molecular dynamics free-energy simulations of the binding contribution to the fidelity of T7 DNA polymerase Source: JOURNAL OF PHYSICAL CHEMISTRY B, 106 (22): 5754-5760 JUN 6 2002 ISSN: 1520-6106	2	0	4	5	1	12	2.00
213. Author(s): WARSHEL, A; CHU, ZT Title: CALCULATIONS OF SOLVATION FREE-ENERGIES IN CHEMISTRY AND BIOLOGY Source: STRUCTURE AND REACTIVITY IN AQUEOUS SOLUTION ACS SYMPOSIUM SERIES, 568: 71-94 1994 ISSN: 0097-6156	1	0	0	0	0	12	0.92
214. Author(s): PARSON, WW; CREIGHTON, S; WARSHEL, A Title: CALCULATIONS OF CHARGE-TRANSFER TRANSITION ENERGIES AND SPECTROSCOPIC PROPERTIES OF A MOLECULAR-CRYSTAL - METHYLBACTERIOPHEOPHORBIIDE-A Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 111 (12): 4277-4284 JUN 7 1989 ISSN: 0002-7863	1	0	0	0	0	12	0.63
215. Author(s): WARSHEL, A; RUSSELL, S; SUSSMAN, F Title: COMPUTER-SIMULATION OF ENZYMATIC-REACTIONS Source: ISRAEL JOURNAL OF CHEMISTRY, 27 (2): 217-224 1986 ISSN: 0021-2148	1	0	0	0	0	12	0.57
216. Author(s): BROMBERG, A; MUSZKAT, KA; WARSHEL, A Title: OXIDATION OF 4A,4B-DIHYDROPHENANTHRENE .4. KINETIC ISOTOPE EFFECT OF DEUTERIUM IN PROPAGATION AND INITIATION STEPS Source: JOURNAL OF CHEMICAL PHYSICS, 52 (11): 5952-& 1970 ISSN: 0021-9606	0	0	0	0	0	12	0.32
217. Author(s): LIANG, R; SCHNEPP, O; WARSHEL, A Title: RESONANCE RAMAN-SPECTRUM OF AZULENE Source: CHEMICAL PHYSICS, 34 (1): 17-27 1978 ISSN: 0301-0104	0	0	0	0	0	11	0.37
218. Author(s): Kato, M; Pislakov, AV; Warshel, A Title: The barrier for proton transport in aquaporins as a challenge for electrostatic models: The role of protein relaxation in mutational calculations Source: PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS, 64 (4): 829-844 SEP 1 2006 ISSN: 0887-3585				2	8	10	5.00
219. Author(s): Madura, JD; Nakajima, Y; Hamilton, RM; et al. Title: Calculations of the electrostatic free energy contributions to the binding free energy of sulfonamides to carbonic anhydrase Source: STRUCTURAL CHEMISTRY, 7 (2): 131-138 APR 1996 ISSN: 1040-0400	0	1	0	1	0	10	0.83
220. Author(s): WARSHEL, A; AQVIST, J Title: ELECTROSTATIC CORRELATION OF STRUCTURE AND FUNCTION IN PROTEINS Source: CHEMICA SCRIPTA, 29A: 75-83 SEP 1989	1	1	0	0	0	10	0.53

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
ISSN: 0004-2056							
221.	0	0	0	0	0	10	0.40
Author(s): WARSHEL, A; CHURG, AK Title: CONVERTING STRUCTURAL-CHANGES UPON OXIDATION OF CYTOCHROME-C TO ELECTROSTATIC REORGANIZATION ENERGY Source: JOURNAL OF MOLECULAR BIOLOGY, 168 (3): 693-697 1983 ISSN: 0022-2836							
222.	0	0	0	0	0	10	0.27
Author(s): WARSHEL, A Title: ANHARMONICITY IN CRYSTAL VIBRATIONS Source: JOURNAL OF CHEMICAL PHYSICS, 54 (12): 5324-& 1971 ISSN: 0021-9606							
223.				0	9	9	4.50
Author(s): Warshel, A; Sharma, PK; Kato, M; et al. Title: Modeling electrostatic effects in proteins Source: BIOCHIMICA ET BIOPHYSICA ACTA-PROTEINS AND PROTEOMICS, 1764 (11): 1647-1676 NOV 2006 ISSN: 1570-9639							
224.	1	1	2	0	1	9	0.90
Author(s): Papazyan, A; Warshel, A Title: Effect of solvent discreteness on solvation Source: JOURNAL OF PHYSICAL CHEMISTRY B, 102 (27): 5348-5357 JUL 2 1998 ISSN: 1089-5647							
225.	0	1	0	0	0	9	0.27
Author(s): DAUBER, P; BRITH, M; HULER, E; et al. Title: VIBRONIC STRUCTURE OF CRYSTALLINE ETHYLENE Source: CHEMICAL PHYSICS, 7 (1): 108-115 1975 ISSN: 0301-0104							
226.				3	5	8	4.00
Author(s): Olsson, MHM; Warshel, A Title: Monte Carlo simulations of proton pumps: On the working principles of the biological valve that controls proton pumping in cytochrome c oxidase Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA, 103 (17): 6500-6505 APR 25 2006 ISSN: 0027-8424							
227.		0	2	4	2	8	2.00
Author(s): Parson, WW; Warshel, A Title: Dependence of photosynthetic electron-transfer kinetics on temperature and energy in a density-matrix model Source: JOURNAL OF PHYSICAL CHEMISTRY B, 108 (29): 10474-10483 JUL 22 2004 ISSN: 1520-6106							
228.	0	2	1	0	0	8	1.00
Author(s): Jen, CF; Warshel, A Title: Microscopic based density matrix treatments of electron-transfer reactions in condensed phases Source: JOURNAL OF PHYSICAL CHEMISTRY A, 103 (51): 11378-11386 DEC 23 1999 ISSN: 1089-5639							
229.			0	4	3	7	2.33
Author(s): Kato, M; Warshel, A Title: Through the channel and around the channel: Validating and comparing microscopic approaches for the evaluation of free energy profiles for ion penetration through ion channels Source: JOURNAL OF PHYSICAL CHEMISTRY B, 109 (41): 19516-19522 OCT 20 2005 ISSN: 1520-6106							
230.	0	1	0	2	0	7	0.88
Author(s): Strajbl, M; Florian, J; Warshel, A Title: Ab initio/LD studies of chemical reactions in solution: Reference free-energy surfaces for acylation reactions occurring in serine and cysteine proteases Source: INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, 77 (1): 44-53 MAR 5 2000 ISSN: 0020-7608							
231.	0	0	0	0	0	7	0.37
Author(s): CHU, ZT; WARSHEL, A; PARSON, WW Title: MICROSCOPIC SIMULATION OF QUANTUM DYNAMICS AND NUCLEAR TUNNELING IN BACTERIAL REACTION CENTERS Source: PHOTOSYNTHESIS RESEARCH, 22 (1): 39-46 OCT 1989 ISSN: 0166-8595							
232.				0	6	6	3.00
Author(s): Klahn, M; Rosta, E; Warshel, A Title: On the mechanism of hydrolysis of phosphate monoesters dianions in solutions and proteins							

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 128 (47): 15310-15323 NOV 29 2006 ISSN: 0002-7863							
233.	0	1	3	1	1	6	1.20
Author(s): Trajbl, M; Hong, GY; Warshel, A Title: Ab initio QM/MM simulation with proper sampling: "First principle" calculations of the free energy of the autodissociation of water in aqueous solution Source: JOURNAL OF PHYSICAL CHEMISTRY B, 106 (51): 13333-13343 DEC 26 2002 ISSN: 1520-6106							
234.	0	0	1	0	0	6	0.75
Author(s): Mehler, EL; Warshel, A Title: Comment on "A fast and simple method to calculate protonation states in proteins" Source: PROTEINS-STRUCTURE FUNCTION AND GENETICS, 40 (1): 1-3 JUL 1 2000 ISSN: 0887-3585							
235.	0	0	0	0	0	6	0.26
Author(s): HWANG, JK; WARSHEL, A Title: SEMICLASSICAL SIMULATIONS OF THE SPECTRA OF ANHARMONIC MOLECULES - PROBLEMS AND ALTERNATIVES Source: CHEMICAL PHYSICS LETTERS, 115 (3): 281-285 1985 ISSN: 0009-2614							
236.				1	4	5	2.50
Author(s): Xiang, Y; Oelschlaeger, P; Florian, J; et al. Title: Simulating the effect of DNA polymerase mutations on transition-state energetics and fidelity: Evaluating amino acid group contribution and allosteric coupling for ionized residues in human pol beta Source: BIOCHEMISTRY, 45 (23): 7036-7048 JUN 13 2006 ISSN: 0006-2960							
237.		1	1	2	1	5	1.25
Author(s): Shurki, A; Strajbl, M; Schutz, CN; et al. Title: Electrostatic basis for bioenergetics Source: ENERGETICS OF BIOLOGICAL MACROMOLECULES, PT E METHODS IN ENZYMOLOGY, 380: 52-84 2004 ISSN: 0076-6879							
238.	0	1	0	3	1	5	1.00
Author(s): Warshel, A; Villa-Freixa, J Title: Comment on "Effect of active site mutation Phe93 -> Trp in the horse liver alcohol dehydrogenase enzyme on catalysis: A molecular dynamics study" Source: JOURNAL OF PHYSICAL CHEMISTRY B, 107 (44): 12370-12371 NOV 6 2003 ISSN: 1520-6106							
239.	0	1	1	0	0	5	0.62
Author(s): Warshel, A Title: Perspective on "The energetics of enzymatic reactions" - Warshel A (1978) Proc Natl Acad Sci USA 75 : 5250 Source: THEORETICAL CHEMISTRY ACCOUNTS, 103 (3-4): 337-339 FEB 2000 ISSN: 1432-881X							
240.	0	0	0	0	0	5	0.15
Author(s): HULER, E; WARSHEL, A Title: CONSISTENT CALCULATION OF LATTICE-DYNAMICS USING SEMIEMPIRICAL POTENTIAL FUNCTIONS Source: CHEMICAL PHYSICS, 8 (1-2): 239-244 1975 ISSN: 0301-0104							
241.	0	0	0	0	0	5	0.15
Author(s): SCHLESSI.J; WARSHEL, A Title: CALCULATIONS OF CD AND CPL SPECTRA AS A TOOL FOR EVALUATION OF CONFORMATIONAL DIFFERENCES BETWEEN GROUND AND EXCITED-STATES OF CHIRAL MOLECULES Source: CHEMICAL PHYSICS LETTERS, 28 (3): 380-383 1974 ISSN: 0009-2614							
242.		1	0	2	1	4	1.00
Author(s): Olsson, MHM; Siegbahn, PEM; Warshel, A Title: Simulating large nuclear quantum mechanical corrections in hydrogen atom transfer reactions in metalloenzymes Source: JOURNAL OF BIOLOGICAL INORGANIC CHEMISTRY, 9 (1): 96-99 JAN 2004 ISSN: 0949-8257							
243.	0	0	1	0	0	4	0.36
Author(s): Warshel, A; Chu, ZT; Parson, WW Title: Two-dimensional free energy surfaces for primary electron transfer in a photosynthetic reaction center Source: CHEMICAL PHYSICS LETTERS, 265 (1-2): 293-296 JAN 31							

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
1997 ISSN: 0009-2614							
244. Author(s): Hong, GY; Rosta, E; Warshel, A Title: Using the constrained DFT approach in generating diabatic surfaces and off diagonal empirical valence bond terms for modeling reactions in condensed phases Source: JOURNAL OF PHYSICAL CHEMISTRY B, 110 (39): 19570-19574 OCT 5 2006 ISSN: 1520-6106				0	3	3	1.50
245. Author(s): Kato, M; Warshel, A Title: Using a charging coordinate in studies of ionization induced partial unfolding Source: JOURNAL OF PHYSICAL CHEMISTRY B, 110 (23): 11566-11570 JUN 15 2006 ISSN: 1520-6106				1	2	3	1.50
246. Author(s): Braun-Sand, S; Olsson, MHM; Warshel, A Title: Computer modeling of enzyme catalysis and its relationship to concepts in physical organic chemistry Source: ADVANCES IN PHYSICAL ORGANIC CHEMISTRY, VOL 40 ADVANCES IN PHYSICAL ORGANIC CHEMISTRY, 40: 201-245 2005 ISSN: 0065-3160			0	2	1	3	1.50
247. Author(s): Sucato, CA; Upton, TG; Kashemirov, BA; et al. Title: Modifying the beta,gamma leaving-group bridging oxygen alters nucleotide incorporation efficiency, fidelity, and the catalytic mechanism of DNA polymerase beta Source: BIOCHEMISTRY, 46 (2): 461-471 JAN 16 2007 ISSN: 0006-2960					2	2	2.00
248. Author(s): Burykin, A; Warshel, A Title: Membranes assembled from narrow carbon nanotubes block proton transport and can form effective nano-filtration devices Source: JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, 3 (2): 237-242 APR 2006 ISSN: 1546-1955				1	1	2	1.00
249. Author(s): Warshel, A Title: Inverting the selectivity of aquaporin 6: Gating versus direct electrostatic interaction Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA, 102 (6): 1813-1814 FEB 8 2005 ISSN: 0027-8424			0	2	0	2	0.67
250. Author(s): Shurki, A; Villa, J; Warshel, A Title: How important is the steric contribution (NAC) to enzyme catalysis? Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 223: 268-PHYS Part 2 APR 7 2002 ISSN: 0065-7727	0	0	0	1	1	2	0.33
251. Author(s): Villa, J; Bentzien, J; Gonzalez-Lafont, A; et al. Title: Effective way of modeling chemical catalysis: Empirical valence bond picture of role of solvent and catalyst in alkylation reactions Source: JOURNAL OF COMPUTATIONAL CHEMISTRY, 21 (8): 607-625 JUN 2000 ISSN: 0192-8651	0	0	0	0	1	2	0.25
252. Author(s): Florian, J; Warshel, A Title: Quantum-chemical insights into mechanisms of the nonenzymatic hydrolysis of phosphate monoesters Source: PHOSPHORUS SULFUR AND SILICON AND THE RELATED ELEMENTS, 146: 525-528 1999 ISSN: 1042-6507	1	0	0	1	0	2	0.22
253. Author(s): Liu, HB; Warshel, A Title: The catalytic effect of dihydrofolate reductase and its mutants is determined by reorganization energies Source: BIOCHEMISTRY, 46 (20): 6011-6025 MAY 22 2007 ISSN: 0006-2960					1	1	1.00
254. Author(s): Warshel, A; Sharma, PK; Chu, ZT; et al. Title: Electrostatic contributions to binding of transition state analogues can be very different from the corresponding contributions to catalysis: Phenolates binding to the oxyanion hole of ketosteroid					1	1	1.00

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
isomerase							
Source: BIOCHEMISTRY, 46 (6): 1466-1476 FEB 13 2007							
ISSN: 0006-2960							
255. Author(s): Warshel, A; Villa, J; Strajbl, M; et al.	0	0	0	0	1	1	0.14
Title: Using computer simulations to elucidate the origin of enzyme catalysis.							
Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 221: 49-COMP Part 1 APR 1 2001							
ISSN: 0065-7727							
256. Author(s): Sham, YY; Muegge, I; Warshel, N	0	0	1	0	0	1	0.11
Title: Effect of protein relaxation on charge-charge interaction and dielectric constants in protein.							
Source: BIOPHYSICAL JOURNAL, 76 (1): A198-A198 Part 2 JAN 1999							
ISSN: 0006-3495							
257. Author(s): WARSHEL, A	0	0	1	0	0	1	0.06
Title: COMPUTER-SIMULATIONS OF CHARGE SEPARATION PROCESSES IN MODEL COMPOUNDS AND BACTERIAL REACTION CENTERS							
Source: PHOTOSYNTHESIS RESEARCH, 34 (1): 91-91 OCT 1992							
ISSN: 0166-8595							
258. Author(s): WARSHEL, A	0	0	0	0	1	1	0.05
Title: SIMULATIONS OF CHEMICAL-REACTIONS IN SOLUTIONS AND IN ENZYMES							
Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 197: 101-PHYS APR 9 1989							
ISSN: 0065-7727							
259. Author(s): KING, G; WARSHEL, A	0	0	0	0	0	1	0.05
Title: THE SURFACE CONSTRAINT ALL-ATOM SOLVENT MODEL							
Source: BIOPHYSICAL JOURNAL, 49 (2): A491-A491 Part 2 FEB 1986							
ISSN: 0006-3495							
260. Author(s): HWANG, JK; WARSHEL, A	0	0	0	0	0	1	0.04
Title: A SHORTCUT FOR MULTIDIMENSIONAL QUANTIZATION - THE AVERAGE PARTIAL ACTIONS METHOD							
Source: CHEMICAL PHYSICS LETTERS, 118 (3): 289-292 1985							
ISSN: 0009-2614							
261. Author(s): Liu, HB; Warshel, A					0	0	0.00
Title: Origin of the temperature dependence of isotope effects in enzymatic reactions: The case of dihydrofolate reductase							
Source: JOURNAL OF PHYSICAL CHEMISTRY B, 111 (27): 7852-7861 JUL 12 2007							
ISSN: 1520-6106							
262. Author(s): Sharma, PK; Chu, ZT; Olsson, MHM; et al.					0	0	0.00
Title: A new paradigm for electrostatic catalysis of radical reactions in vitamin B-12 enzymes							
Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA, 104 (23): 9661-9666 JUN 5 2007							
ISSN: 0027-8424							
263. Author(s): Roca, M; Messer, B; Warshel, A					0	0	0.00
Title: Electrostatic contributions to protein stability and folding energy							
Source: FEBS LETTERS, 581 (10): 2065-2071 MAY 15 2007							
ISSN: 0014-5793							
264. Author(s): Olsson, MHM; Slegbahn, PEM; Blomberg, MRA; et al.					0	0	0.00
Title: Exploring pathways and barriers for coupled ET/PT in cytochrome c oxidase: A general framework for examining energetics and mechanistic alternatives							
Source: BIOCHIMICA ET BIOPHYSICA ACTA-BIOENERGETICS, 1767 (3): 244-260 MAR 2007							
ISSN: 0005-2728							
265. Author(s): Martinek, V; Bren, U; Goodman, MF; et al.					0	0	0.00
Title: DNA polymerase beta catalytic efficiency mirrors the Asn279-dCTP H-bonding strength							
Source: FEBS LETTERS, 581 (4): 775-780 FEB 20 2007							
ISSN: 0014-5793							

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
266. Author(s): Oelschlaeger, P; Klahn, M; Beard, WA; et al. Title: Magnesium-cationic dummy atom molecules enhance representation of DNA polymerase beta in molecular dynamics simulations: Improved accuracy in studies of structural features and mutational effects Source: JOURNAL OF MOLECULAR BIOLOGY, 366 (2): 687-701 FEB 16 2007 ISSN: 0022-2836					0	0	0.00
267. Author(s): Warshel, A Title: Using computer simulations to establish the key role of electrostatic preorganization energy in enzyme catalysis Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 230: U541-U541 83-BIOL AUG 28 2005 ISSN: 0065-7727			0	0	0	0	0.00
268. Author(s): Rosta, E; Warshel, A Title: Ab initio free energies of enzymatic reactions using model potentials. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 229: U743-U743 270-PHYS Part 2 MAR 13 2005 ISSN: 0065-7727			0	0	0	0	0.00
269. Author(s): Kato, M; Warshel, A Title: Exploring microscopic simulation methods for ion transport energetics in gramicidin. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 229: U776-U777 485-PHYS Part 2 MAR 13 2005 ISSN: 0065-7727			0	0	0	0	0.00
270. Author(s): Braun-Sand, S; Warshel, A Title: Simulating the primary proton transport event in bacteriorhodopsin Source: BIOPHYSICAL JOURNAL, 88 (1): 507A-507A Part 2 Suppl. S JAN 2005 ISSN: 0006-3495			0	0	0	0	0.00
271. Author(s): Olsson, MHM; Warshel, A Title: Simulating redox coupled proton transfer in cytochrome c oxidase Source: BIOPHYSICAL JOURNAL, 88 (1): 548A-548A Part 2 Suppl. S JAN 2005 ISSN: 0006-3495			0	0	0	0	0.00
272. Author(s): Braun-Sand, S; Warshel, A Title: Studies of proton translocations in biological systems. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 228: U189-U189 109-BIOL Part 1 AUG 22 2004 ISSN: 0065-7727		0	0	0	0	0	0.00
273. Author(s): Warshel, A Title: Challenges and advances in QM/MM methods for studies of energetics and dynamics of biological systems. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 228: U235-U235 232-PHYS Part 2 AUG 22 2004 ISSN: 0065-7727		0	0	0	0	0	0.00
274. Author(s): Warshel, A Title: Simulating phosphate hydrolysis in key biological reactions. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 228: U308-U308 728-PHYS Part 2 AUG 22 2004 ISSN: 0065-7727		0	0	0	0	0	0.00
275. Author(s): Olsson, MHM; Warshel, A Title: Simulations of the large kinetic isotope effect and the temperature dependence of the hydrogen atom transfer in lipoxxygenase. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 227: U312-U313 355-PHYS Part 2 MAR 28 2004 ISSN: 0065-7727		0	0	0	0	0	0.00
276. Author(s): Burykin, A; Warshel, A Title: What really prevents proton transport through aquaporin? Charge self-energy versus proton wire proposals Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 227: U319-U319 397-PHYS Part 2 MAR 28 2004 ISSN: 0065-7727		0	0	0	0	0	0.00

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
277. Author(s): Rosta, E; Warshel, A Title: Ab initio QM/MM simulation with proper sampling: A study of the reaction of orotidine-5 '-monophosphate decarboxylase Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 227: U320-U320 407-PHYS Part 2 MAR 28 2004 ISSN: 0065-7727		0	0	0	0	0	0.00
278. Author(s): Kato, N; Warshel, A Title: Calculations of binding free energies for chorismate mutase inhibitors. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 227: U322-U323 422-PHYS Part 2 MAR 28 2004 ISSN: 0065-7727		0	0	0	0	0	0.00
279. Author(s): Warshel, A Title: Implicit and explicit electrostatic models for structure function correlation of biomolecules. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 225: U745-U745 087-COMP Part 1 MAR 2003 ISSN: 0065-7727	0	0	0	0	0	0	0.00
280. Author(s): Rosta, E; Warshel, A Title: Analytical derivatives for langevin dipoles solvation model Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 225: U771-U771 249 Part 1 MAR 2003 ISSN: 0065-7727	0	0	0	0	0	0	0.00
281. Author(s): Strajbl, M; Hong, GY; Warshel, A Title: Ab-initio QM/MM calculations of free energies Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 225: U771-U771 250 Part 1 MAR 2003 ISSN: 0065-7727	0	0	0	0	0	0	0.00
282. Author(s): Hong, GY; Strajbl, M; Warshel, A Title: QM(CDFT)/MM molecular dynamic free energy studies of enzymatic reactions Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 225: U771-U771 25 Part 1 MAR 2003 ISSN: 0065-7727	0	0	0	0	0	0	0.00
283. Author(s): Burykin, A; Warshel, A Title: What really prevents proton transport through aquaporin? Charge selfenergy versus proton wire proposals. Source: BIOPHYSICAL JOURNAL, 86 (1): 612A-612A Part 2 Suppl. S JAN 2004 ISSN: 0006-3495		0	0	0	0	0	0.00
284. Author(s): Strajbl, M; Shurky, A; Warshel, A Title: Energetics of ATP synthase: Conversion of the conformational changes to electrostatic energies. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 225: U455-U455 147-PHYS Part 2 MAR 2003 ISSN: 0065-7727	0	0	0	0	0	0	0.00
285. Author(s): Burykin, A; Kato, M; Warshel, A Title: Simulating ion current and selectivity in realistic models of the KcsA potassium channel. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 225: U462-U462 193-PHYS Part 2 MAR 2003 ISSN: 0065-7727	0	0	0	0	0	0	0.00
286. Author(s): Warshel, A Title: Ion selectivity in ion channel as a challenge for electrostatic modeling of proteins. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 225: U468-U468 234-PHYS Part 2 MAR 2003 ISSN: 0065-7727	0	0	0	0	0	0	0.00
287. Author(s): Shurki, A; Strajbl, M; Warshel, A Title: ATP synthase - An energy based insight. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 225: U516-U516 452-PHYS Part 2 MAR 2003 ISSN: 0065-7727	0	0	0	0	0	0	0.00
288. Author(s): Warshel, Y Title: 'Dear BBC': Children, television storytelling and the public sphere Source: JOURNAL OF COMMUNICATION, 53 (4): 735-737 DEC 2003	0	0	0	0	0	0	0.00

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
ISSN: 0021-9916							
289.	0	0	0	0	0	0	0.00
Author(s): Shaw, WB; Gragg, DJ; Warshel, EV; et al. Title: ASCP-BOR honors 50-year certificants Source: LABORATORY MEDICINE, 34 (5): 6-7 MAY 2003 ISSN: 0007-5027							
290.	0	0	0	0	0	0	0.00
Author(s): Florian, J; Shurki, A; Warshel, A Title: Empirical valence bond strategies for phosphoryl and nucleotidyl transfer reactions. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 224: 070-COMP Part 1 AUG 18 2002 ISSN: 0065-7727							
291.	0	0	0	0	0	0	0.00
Author(s): Warshel, A; Villa, J; Glennon, T Title: How does GAP catalyze the GTPase reaction of RAS? Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 223: 041-PHYS Part 2 APR 7 2002 ISSN: 0065-7727							
292.	0	0	0	0	0	0	0.00
Author(s): Florin, J; Goodman, MF; Warshel, A Title: Computer simulations of the replication fidelity of DNA polymerase T7. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 223: 168-PHYS Part 2 APR 7 2002 ISSN: 0065-7727							
293.	0	0	0	0	0	0	0.00
Author(s): Warshel, A Title: Electrostatic aspects of structure-function correlation in biomolecules; From PKA calculations to studies of signal transduction and ion channels. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 223: 182-PHYS Part 2 APR 7 2002 ISSN: 0065-7727							
294.	0	0	0	0	0	0	0.00
Author(s): Schutz, CN; Warshel, A Title: What are the dielectric "constants" of proteins and how to validate electrostatic models? Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 223: 376-PHYS Part 2 APR 7 2002 ISSN: 0065-7727							
295.	0	0	0	0	0	0	0.00
Author(s): Burykin, A; Schutz, CN; Villa, J; et al. Title: On-the-fly simulations of ion current in realistic models of ion channels: The KcsA potassium channel Source: BIOPHYSICAL JOURNAL, 82 (1): 1011 Part 2 JAN 2002 ISSN: 0006-3495							
296.	0	0	0	0	0	0	0.00
Author(s): Warshel, A; Villa, J; Shurki, A; et al. Title: Pushing the frontiers of QM/MM methods for studies of energetics and dynamics in large systems. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 222: 10-COMP Part 1 AUG 2001 ISSN: 0065-7727							
297.	0	0	0	0	0	0	0.00
Author(s): Warshel, A; Jen, CY; Villa, J Title: Does dynamically driven tunneling effects contribute in a major way to enzyme catalysis? Source: BIOPHYSICAL JOURNAL, 80 (1): 114 Part 2 JAN 2001 ISSN: 0006-3495							
298.	0	0	0	0	0	0	0.00
Author(s): Jen, CY; Villa, J; Warshel, A Title: Dynamically driven tunneling effects are unlikely to contribute in a major way to enzyme catalysis. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 220: 21-PHYS Part 2 AUG 20 2000 ISSN: 0065-7727							
299.	0	0	0	0	0	0	0.00
Author(s): Sham, YY; Muegge, I; Warshel, A Title: Simulating proton translocations in proteins: Probing proton transfer pathways in the Rhodobacter sphaeroides reaction center. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 220: 146-PHYS Part 2 AUG 20 2000 ISSN: 0065-7727							
300.	0	0	0	0	0	0	0.00
Author(s): Warshel, A Title: Implicit and explicit models for calculations of electrostatic energies in proteins.							

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
	Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 219: 199-PHYS Part 2 MAR 26 2000 ISSN: 0065-7727						
301.	0	0	0	0	0	0	0.00
	Author(s): Warshel, A; Chu, ZT; Tao, H; et al. Title: Examining methods for calculations of binding free energies: LRA, LIE and PDLD/S-LRA calculations of ligands binding to proteins Source: BIOPHYSICAL JOURNAL, 78 (1): 1965Pos Part 2 JAN 2000 ISSN: 0006-3495						
302.	0	0	0	0	0	0	0.00
	Author(s): Warshel, A; Sham, YY; Muegge, I Title: Simulating proton translocations in proteins: Probing proton transfer pathways in the Rhodobacter sphaeroides reaction center. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 218: 80-COMP Part 1 AUG 22 1999 ISSN: 0065-7727						
303.	0	0	0	0	0	0	0.00
	Author(s): Warshel, A Title: Simulations of chemical reactions in proteins and solutions by ab initio and related approaches. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 218: 180-COMP Part 1 AUG 22 1999 ISSN: 0065-7727						
304.	0	0	0	0	0	0	0.00
	Author(s): Glennon, TM; Warshel, A Title: A computational study of the catalytic reaction of ribonuclease A Source: BIOPHYSICAL JOURNAL, 76 (1): A180-A180 Part 2 JAN 1999 ISSN: 0006-3495						
305.	0	0	0	0	0	0	0.00
	Author(s): Warshel, A Title: Probing the energetics and dynamics of enzymatic reactions. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 216: 500-PHYS Part 2 AUG 23 1998 ISSN: 0065-7727						
306.	0	0	0	0	0	0	0.00
	Author(s): Warshel, A Title: Elucidating the origin of transition state stabilization in enzymatic reactions. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 215: 049-COMP Part 1 APR 2 1998 ISSN: 0065-7727						
307.	0	0	0	0	0	0	0.00
	Author(s): Warshel, A Title: Electronic structure calculations of chemical reactions in proteins and solutions. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 215: 414-PHYS Part 2 APR 2 1998 ISSN: 0065-7727						
308.	0	0	0	0	0	0	0.00
	Author(s): Warshel, A Title: Ab initio QM/MM approaches of studying chemical reactions in proteins and solutions: Strategies, problems and perspectives. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 214: 69-COMP Part 1 SEP 7 1997 ISSN: 0065-7727						
309.	0	0	0	0	0	0	0.00
	Author(s): Warshel, A Title: Consistent calculations of electrostatic energies in proteins and solutions. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 214: 191-COMP Part 1 SEP 7 1997 ISSN: 0065-7727						
310.	0	0	0	0	0	0	0.00
	Author(s): Papazyan, A; Warshel, A Title: A stringent test of the cavity concept in continuum dielectrics. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 214: 218-COMP Part 1 SEP 7 1997 ISSN: 0065-7727						
311.	0	0	0	0	0	0	0.00
	Author(s): Florian, J; Warshel, A Title: Langevin dipoles model for ab initio calculations of chemical processes in solution: Parametrization and application to phosphate ester hydrolysis and conformational analysis in aqueous solution. Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 214: 85-PHYS Part 2 SEP 7 1997 ISSN: 0065-7727						

	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
312. Author(s): Bunte, SW; Jensen, GM; Warshel, A; et al. Title: Combined ab initio and electrostatic calculations of tryptophan-191 oxidation in compound ES of cytochrome c peroxidase Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 213: 306-PHYS Part 2 APR 13 1997 ISSN: 0065-7727	0	0	0	0	0	0	0.00
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315. Author(s): Bunte, SW; Jensen, GM; Warshel, A; et al. Title: Combined ab initio and electrostatic calculations of tryptophan-191 oxidation in compound ES of cytochrome C peroxidase Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 211: 506-INOR Part 1 MAR 24 1996 ISSN: 0065-7727	0	0	0	0	0	0	0.00
316. Author(s): WARSHEL, A Title: COMPUTER-SIMULATION OF PROTON-TRANSFER REACTIONS IN ENZYMES AND THE ELECTROSTATIC NATURE OF CATALYTIC HYDROGEN-BONDS Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 210: 147-PHYS Part 2 AUG 20 1995 ISSN: 0065-7727	0	0	0	0	0	0	0.00
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320. Author(s): WARSHEL, A Title: COMPUTER-SIMULATION OF ELECTRON-TRANSFER AND PROTON-TRANSFER IN PROTEINS AND SOLUTIONS Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 206: 65-PHYS Part 2 AUG 22 1993 ISSN: 0065-7727	0	0	0	0	0	0	0.00
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	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
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326. Author(s): WARSHEL, A Title: EVALUATING CATALYTIC FREE-ENERGY IN ENZYMES Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 194: 7-BIOL AUG 30 1987 ISSN: 0065-7727	0	0	0	0	0	0	0.00
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333. Author(s): WARSHEL, A; SUSSMAN, F Title: TOWARD COMPUTER-AIDED SITE-DIRECTED MUTAGENESIS Source: BIOPHYSICAL JOURNAL, 49 (2): A529-A529 Part 2 FEB 1986 ISSN: 0006-3495	0	0	0	0	0	0	0.00
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	2003	2004	2005	2006	2007	Total	Average Citations per Year
	1364	1399	1267	1711	1059	22,176	554.40
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