ROI BAER: CURRICULUM VITAE

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Personal Information

Born Jerusalem September 30, 1961; Raised mostly in Rehovoth, married +2, Lives in 2 Mishkan Shiloh, Jerusalem, Israel (Cellular: +972-54-7958017).

Academia

1979-1982	**B.Sc. Mathematics and Physics,** The Hebrew University of Jerusalem
1991-1993	**M.Sc. Theoretical Chemistry, Summa Cum Laude, (with Professor Ronnie Kosloff)** The Hebrew University of Jerusalem.
1994-1996	**Ph.D. Theoretical Chemistry, (with Professor Ronnie Kosloff)** The Hebrew University of Jerusalem.
1996-1998	**Postdoc, Theoretical Chemistry, (with Professor Martin Head-Gordon)** University of California, Berkeley, CA, USA.

Faculty positions

1998	**Senior Lecturer,** The Hebrew University of Jerusalem
2002	**Associate Professor,** The Hebrew University of Jerusalem
2006	**Full Professor,** The Hebrew University of Jerusalem
2005-2006	**Visiting Professor,** University of California at Los Angeles
2006-2007	**Chair, Dept. Physical Chemistry,** The Hebrew University of Jerusalem
2006-	**Director of The Fritz Haber Center for Molecular Dynamics,** The Hebrew University of Jerusalem
2008	**Visiting Professor (delivered a semester course on DFT),** University of Southern California at Los Angeles
2012-2015	**Co-director of the Hoffman Leadership and Responsibility Program** Hebrew University of Jerusalem

Honors, Editorial, and Advisory Boards

1995	Wolf Foundation prize for Ph.D. students
1996	The Fritz Haber research center prize
2000	The Josepha and Leonid Olschwang prize, Israel Academy of Science
2001	Noted “Excellent Teacher” of the Science Faculty
2003	Invited Editor of Special Issue on Computational Chemistry; Israel Journal of Chemistry
2006-2007	Editorial Advisory Board “Physical Chemistry-Chemical Physics”
2007	Noted “Excellent Teacher” of the Science Faculty
2008-today	Member of the Fellowships Committee of Minerva Steiftung in the Max Planck Society
2010-2014	Member of Editorial Committee of Annual Reviews of Physical Chemistry
2010	Noted “Excellent Teacher” of the Science Faculty
2011	Voted chair of 2015 Gordon Conference on Time Dependent Density Functional Theory
2011	Guest Editor for Special Issue on "Open Problems in Time dependent density functional Theory", for “Chemical Physics” (together with L. Kronik and S. Kuemmel)
2011-2012	Associate Editor of Theoretical Chemistry Accounts (Springer)
2013-2015	Member of JPC Editorial Advisory Board
2013	The Klachky Prize for the Advancement of the Frontiers of Science
2015	Ratner Family Chair in Chemistry
2015-16	Visiting Pitzer Professorship, University of California Berkeley
2015-16	Heising-Simons Visiting Fellow of the Kavli Energy Nanoscience Institute at UC Berkeley
2018	Rector’s Prize for Excellence in Teaching and Research

Teaching at the Hebrew University

	“Introduction to Chemical Bonding” (Under-Grad, 6 hrs/wk)
	“Theoretical Methods and Techniques in Chemistry” (Graduate, 4 hrs/wk)
	“Physical Chemistry III” (Graduate, with Professors Avinoam Ben-Shaul and Sanford Ruhman)
	“Density Functional Theory” (Graduate, 4 hrs/wk)
	Advanced Laboratory in Chemical Physics (the theoretical chapter)

Conference organization

2002	Israel Theochem
2007	Co-chair Safed Summer School on DFT
2007	Chair of the Gentner Symposium on TDDFT
2013	Co-Chair of School and workshop in Natural and Manmade Light Harvesting systems
2015	Co-organizer, The Batsheva de Rothschild Seminar on Molecular Electronics 2015
2017	Co-Chair CECAM Workshop Stochastic Methods in Electronic Structure Theory (Tel Aviv)
2018	Chair of “Jerusalem Nonadiabatica 2018” – conference on the theory of nonadiabatic processes.

List of Publications

No.	PUBLICATION
145	Y. CYTTER, E. RABANI, D. NEUHAUSER AND **R. BAER**, STOCHASTIC DENSITY FUNCTIONAL THEORY AT FINITE TEMPERATURES. ARXIV:1801.02163 [COND-MAT.MTRL-SCI] 2018.
144	VLČEK, V. ; RABANI, E. ; NEUHAUSER, D. ; **BAER, R.** STOCHASTIC GW CALCULATIONS FOR MOLECULES. J. CHEM. THEORY COMPUT. 2017, 13, 4997–5003.
143	V. VLČEK, R. BAER,E. RABANI, AND D. NEUHAUSER, "SELF-CONSISTENT BAND-GAP RENORMALIZATION GW". ARXIV PREPRINT ARXIV:1701.02023 2017.
142	NEUHAUSER, D. ; **BAER, R.** ; ZGID, D. STOCHASTIC SELF-CONSISTENT SECOND-ORDER GREEN'S FUNCTION METHOD FOR CORRELATION ENERGIES OF LARGE ELECTRONIC SYSTEMS. J. CHEM. THEORY COMPUT. 2017, 13, 5396−5403
141	TAKESHITA, T. Y. ; DE JONG, W. A. ; NEUHAUSER, D. ; **BAER, R.** ; RABANI, E. STOCHASTIC FORMULATION OF THE RESOLUTION OF IDENTITY: APPLICATION TO SECOND ORDER MØLLER–PLESSET PERTURBATION THEORY. J. CHEM. THEORY COMPUT. 2017, 13, 4605.
140	BUCHMAN, O. ; **BAER, R**. STOCHASTIC METHOD FOR CALCULATING THE GROUND-STATE ONE-BODY DENSITY MATRIX OF TRAPPED BOSE PARTICLES IN ONE DIMENSION. PHYS. REV. A 2017, 96, 033626
139	R. E. HADAD AND **R. BAER** "MINIMALLY-CORRECTED PARTIAL ATOMIC CHARGES FOR NON-COVALENT ELECTROSTATIC INTERACTIONS", MOLEC. PHYS. (IN PRESS) (2017).
138	E. ARNON, E. RABANI, D. NEUHAUSER, AND **R. BAER** "EQUILIBRIUM CONFIGURATIONS OF LARGE NANOSTRUCTURES USING EMBEDDED-SATURATED-FRAGMENT STOCHASTIC DENSITY FUNCTIONAL THEORY", J. CHEM. PHYS. 146, 224111 (2017).
137	LUZON, I. ; JAGTAP, K. ; LIVSHITS, E. ; LIOUBASHEVSKI, O. ; **BAER, R.** ; STRASSER, D. SINGLE-PHOTON COULOMB EXPLOSION OF METHANOL USING BROAD BANDWIDTH ULTRAFAST EUV PULSES. PHYS. CHEM. CHEM. PHYS. 2017, 19, 13488–13495
136	H. ESHET, **R. BAER**, D. NEUHAUSER, E. RABANI "THEORY OF HIGHLY EFFICIENT MULTIEXCITON GENERATION IN TYPE-II NANORODS", NATURE COMM. 7, 13178 (2016).
135	Q. FENG, A. YAMADA, **R. BAER** & B. D. DUNIETZ, "DELETERIOUS EFFECTS OF EXACT EXCHANGE FUNCTIONALS ON PREDICTIONS OF MOLECULAR CONDUCTANCE", J. CHEMICAL THEORY AND COMPUT. 12, 3431-3435 (2016).
134	V. VLCEK, H. R. EISENBERG, G. STEINLE-NEUMANN E. RABANI, D. NEUHAUSER AND **R. BAER**, "SPONTANEOUS CHARGE-CARRIER LOCALIZATION IN EXTENDED ONE-DIMENSIONAL SYSTEMS", PHYS. REV. LETT. 116, 186401 (2016).
133	D. NEUHAUSER, E. RABANI, Y. CYTTER AND **R. BAER** "STOCHASTIC OPTIMALLY-TUNED RANGED-SEPARATED HYBRID DENSITY FUNCTIONAL THEORY", J. J. PHYS. CHEM. 120, 3071 (2016).
132	E. RABANI, **R. BAER**, AND D. NEUHAUSER, "TIME-DEPENDENT STOCHASTIC BETHE-SALPETER APPROACH", PHYS. REV.B 91, 235302 (2015).

No.	PUBLICATION
131	Y. GAO, D. NEUHAUSER, **R. BAER**, E. RABANI, "SUBLINEAR SCALING FOR TIME-DEPENDENT STOCHASTIC DENSITY FUNCTIONAL THEORY", J. CHEM. PHYS. 142, 034106 (2015).
130	V. VLČEK, H. R. EISENBERG, G. STEINLE-NEUMANN, L. KRONIK AND **R. BAER**, "DEVIATIONS FROM PIECEWISE LINEARITY IN THE SOLID-STATE LIMIT WITH APPROXIMATE DENSITY FUNCTIONALS", J. CHEM. PHYS. 142, 034107 (2015)
129	H. R. EISENBERG AND **R. BAER**, "AN EXOTHERMIC MECHANISM FOR THE ABSTRACTION OF HYDROGEN FROM METHANE ON LI-DOPED MGO", J. PHYS. CHEM. C 119, 196−215 (2015).
128	D. NEUHAUSER, Y. GAO, C. ARNTSEN, C. KARSHENAS, E. RABANI AND **R. BAER**, "BREAKING THE THEORETICAL SCALING LIMIT FOR PREDICTING QUASI-PARTICLE ENERGIES: THE STOCHASTIC GW APPROACH", PHYS. REV. LETT. 113, 076402 (2014)
127	A. BARATZ, A. J. WHITE, M. GALPERIN AND **R. BAER**, "LIGHT INDUCED CONDUCTANCE IN A GATED TUNNEL JUNCTION", **5,** 3545-3550, J. PHYS. CHEM. LETT. (2014)
126	Y. CYTTER, D. NEUHAUSER AND **R. BAER**, "METROPOLIS EVALUATION OF THE HARTREE-FOCK EXCHANGE ENERGY", J. CHEM. THEORY COMPUT. (2014).
125	H. ESHET, **R. BAER**, D. NEUHAUSER AND E. RABANI, "MULTIEXCITON GENERATION IN SEEDED NANORODS", J. CHEM. PHYS. LETT. 5, 2580-2585 (2014).
124	D. NEUHAUSER, **R. BAER** AND E. RABANI, "COMMUNICATION: EMBEDDED FRAGMENT STOCHASTIC DENSITY FUNCTIONAL THEORY", J. CHEM. PHYS. 141, 041102 (2014).
123	Q. GE, Y. GAO, **R. BAER**, E. RABANI AND D. NEUHAUSER, "A GUIDED STOCHASTIC ENERGY-DOMAIN FORMULATION OF THE SECOND ORDER MØLLER-PLESSET PERTURBATION THEORY", J. PHYS. CHEM. LETT., 5, 189-185 (2014).
122	D. A. EGGER, S. WEISMANN, S. REFAELY-ABRAMSON, S. SHARIFZADEH, M. DAUTH, **R. BAER**, S. KUMMEL, J. B. NEATON, E. ZOJER, AND L. KRONIK, "OUTER-VALENCE ELECTRON SPECTRA OF PROTOTYPICAL AROMATIC HETEROCYCLES FROM AN OPTIMALLY-TUNED RANGE-SEPARATED HYBRID FUNCTIONAL", J. CHEM. THEORY. COMPUT., DOI:10.1021/CT400956H (2014).
121	**R. BAER** AND D. NEUHAUSER, E. RABANI "SELF-AVERAGING STOCHASTIC KOHN-SHAM DENSITY FUNCTIONAL THEORY", PHYS. REV. LETT. 111, 106402 (2013).
120	S. REFAELY-ABRAMSON, S. SHARIFZADEH, M. JAIN, **R. BAER**, J. B. NEATON, AND L. KRONIK, "GAP RENORMALIZATION OF MOLECULAR CRYSTALS FROM DENSITY FUNCTIONAL THEORY", PHYS. REV. B 88 081204(R) (2013).
119	D. NEUHAUSER, E. RABANI AND **R. BAER** "EXPEDITIOUS STOCHASTIC CALCULATION OF RANDOM-PHASE APPROXIMATION ENERGIES FOR THOUSANDS OF ELECTRONS IN 3 DIMENSIONS", J. PHYS. CHEM. LETT. 4, 1172 − 1176 (2013).
118	D. NEUHAUSER, E. RABANI AND **R. BAER** "EXPEDITIOUS STOCHASTIC APPROACH FOR MP2 ENERGIES IN LARGE ELECTRONIC SYSTEMS", J. CHEM. THEORY COMPUT. 9, PP 24–27 (2012).
117	A. BARATZ, M. GALPERIN AND **R. BAER** "GATE-INDUCED INTRA-MOLECULAR CHARGE-TRANSFER IN A TUNNEL JUNCTION: A NON-EQUILIBRIUM ANALYSIS", J. PHYS. CHEM. C 117, 10257−10263 (2013).

No.	PUBLICATION
116	**R. BAER** AND E. RABANI "COMMUNICATION: BIEXCITON GENERATION RATES IN CDSE NANORODS ARE LENGTH INDEPENDENT", J. CHEM. PHYS. 138, 051102 (2013).
115	G. ZOHAR, **R. BAER** AND E. RABANI "MULTIEXCITON GENERATION IN IV-VI NANOCRYSTALS: THE ROLE OF CARRIER EFFECTIVE MASS, BAND MIXING, AND PHONON EMISSION", J. PHYS. CHEM. LETT. 4, 317-322 (2012).
114	T. STEIN, J. AUTSCHBACH, N. GOVIND, L. KRONIK AND **R.BAER** "CURVATURE AND FRONTIER ORBITAL ENERGIES IN DENSITY FUNCTIONAL THEORY", J. PHYS. CHEM. LETT. 3, 3740 (2012).
113	S. REFAELY-ABRAMSON, S. SHARIFZADEH, N. GOVIND, J. AUTSCHBACH, J. B. NEATON, **R. BAER** AND L. KRONIK, "QUASIPARTICLE SPECTRA FROM A NON-EMPIRICAL OPTIMALLY-TUNED RANGE-SEPARATED HYBRID DENSITY FUNCTIONAL", PHYS. REV. LETT. 22, 226405 (2012).
112	P. K. JAIN, D. GHOSH, **R. BAER**, E. RABANI, AND A. P. ALIVISATOS, "NEAR-FIELD MANIPULATION OF SPECTROSCOPIC SELECTION RULES ON THE NANOSCALE", PROC. NATL. ACAD. SCI., 109, 8016 (2012).
111	L. KRONIK, T. STEIN, S. REFAELY-ABRAMSON AND **R.BAER** "EXCITATION GAPS OF FINITE-SIZED SYSTEMS FROM OPTIMALLY-TUNED RANGE-SEPARATED HYBRID FUNCTIONALS", JCTC, 8, 1515 (2012).
110	A. BARATZ AND **R.BAER** "NON-MECHANICAL CONDUCTANCE SWITCHING IN A REALISTIC MOLECULAR TUNNEL JUNCTION", J. PHYS, CHEM. LETT. 3, 498 (2012).
109	**R. BAER** AND E. RABANI, "EXPEDITIOUS STOCHASTIC CALCULATION OF MULTIEXCITON GENERATION RATES IN SEMICONDUCTOR NANOCRYSTALS", NANO LETT. 12,2123 (2012).
108	S. JACOBI AND **R.BAER** "VARIATIONAL GRAND-CANONICAL ELECTRONIC STRUCTURE OF LI+LI AT ~10,000K WITH SECOND-ORDER PERTURBATION THEORY CORRECTIONS", THEOR. CHEM. ACC. 131, 1113 (2012).
107	**R. BAER** AND D. NEUHAUSER, "MONTE CARLO CALCULATION OF THE EXCHANGE ENERGY", J. CHEM. PHYS., 137,051103 (2012).
106	T.ANSBACHER, H. K. SRIVASTAVA,T. STEIN, **R. BAER**, M. MERKX AND A. SHURKI, "CALCULATION OF TRANSITION DIPOLE MOMENT IN FLUORESCENT PROTEINS — TOWARDS EFFICIENT ENERGY TRANSFER", 14, 4109, PCCP (2012).
105	N. KURITZ,T.STEIN, **R. BAER** AND L. KRONIK, "CHARGE-TRANSFER-LIKE π→π* EXCITATIONS IN TIME-DEPENDENT DENSITY FUNCTIONAL THEORY: A CONUNDRUM AND ITS SOLUTION", J. CHEM. THEORY COMPUT., 7, 240 (2011).
104	S. REFAELY-ABRAMSON, **R.BAER** AND L. KRONIK, "FUNDAMENTAL AND EXCITATION GAPS IN MOLECULES OF RELEVANCE FOR ORGANIC PHOTOVOLTAICS FROM AN OPTIMALLY TUNED RANGE-SEPARATED HYBRID FUNCTIONAL", PHYS. REV. B, 84, 075144 (2011).
103	E. LIVSHITS, R. S. GRANOT AND **R. BAER**, "A DENSITY FUNCTIONAL THEORY FOR STUDYING IONIZATION PROCESSES IN WATER CLUSTERS", J. PHYS. CHEM. A, 115 , 5735 (2011).
102	A. KAROLEWSKI, T. STEIN, **R. BAER** AND S. KÜMMEL, "TAILORING THE OPTICAL GAP IN LIGHT-HARVESTING MOLECULES", J. CHEM. PHYS. 134, 151101 (2011).

No.	PUBLICATION
101	T. STEIN, H. EISENBERG, L. KRONIK AND **R. BAER**, "FUNDAMENTAL GAPS OF FINITE SYSTEMS FROM THE EIGENVALUES OF A GENERALIZED KOHN-SHAM METHOD", PHYS. REV. LETT., 105, 266802 (2010).
100	**R. BAER** AND E. RABANI, "CAN IMPACT EXCITATION EXPLAIN EFFICIENT CARRIER MULTIPLICATION IN CARBON NANOTUBE PHOTODIODES?", NANO LETT. 10 3277 (2010).
99	**R. BAER**, "GROUND STATE DEGENERACIES LEAVE A TOPOLOGICAL SCAR IN THE DENSITY", PHYS. REV. LETT, 104, 073001 (2010)
98	**R. BAER**, E. LIVSHITS AND U. SALZNER, "TUNED RANGE-SEPARATED HYBRIDS IN DENSITY FUNCTIONAL THEORY", ANNU. REV. PHYS. CHEM., 61, 85 (2010).
97	U. SALZNER AND **R. BAER**, "KOOPMANS' SPRINGS TO LIFE", J. CHEM. PHYS. 131, 23110 (2009).
96	T. STEIN, L. KRONIK AND **R. BAER**, "PREDICTION OF CHARGE-TRANSFER EXCITATIONS IN COUMARIN-BASED DYES USING A RANGE-SEPARATED FUNCTIONAL TUNED FROM FIRST PRINCIPLES" J. CHEM. PHYS. **131,** 244119 (2009).
95	A. K. PAUL, S. ADHIKARI, M. BAER AND **R. BAER**, "H2+ PHOTODISSOCIATION BY AN INTENSE PULSED PHOTONIC FOCK-STATE", PHYS REV A **81**, 013412 (2009).
94	J. ANDZELM, B. C. RINDERSPACHER, A. RAWLETT, J. DOUGHERTY, **R. BAER**, N. GOVIND, "PERFORMANCE OF DFT METHODS IN THE CALCULATION OF OPTICAL SPECTRA OF TCF-CHROMOPHORES", J. CHEM. THEO. COMP. 5, 2835(2009)
93	H. EISENBERG AND **R. BAER** , "A NEW GENERALIZED KOHN-SHAM METHOD FOR FUNDAMENTAL BAND-GAPS IN SOLIDS", PCCP, 11, 4674 (2009).
92	E. LIVSHITS, **R. BAER** AND R. KOSLOFF, "THE DELETERIOUS EFFECTS OF LONG-RANGE SELF-REPULSION ON THE DENSITY FUNCTIONAL DESCRIPTION OF O2 STICKING ON ALUMINUM", J. CHEM. PHYS. A, 113, 7521 (2009).
91	**R. BAER** "PREVALENCE OF THE ADIABATIC EXCHANGE-CORRELATION POTENTIAL APPROXIMATION IN TIME-DEPENDENT DENSITY FUNCTIONAL THEORY", J. MOLEC. STRUCT THEOCHEM DOI:10.1016/J.THEOCHEM.2009.04.018 (2009).
90	T. STEIN, L. KRONIK AND **R. BAER** "RELIABLE PREDICTION OF CHARGE TRANSFER EXCITATIONS IN MOLECULAR COMPLEXES USING TIME-DEPENDENT DENSITY FUNCTIONAL THEORY", J. AM. CHEM. SOC. 131, 2818 (2009).
89	A. K. PAUL, S. ADHIKARI, D. MUKHOPADHYAY, G. J. HALÁSZ, Á.VIBÓK, **R. BAER** AND M. BAER, "PHOTODISSOCIATION OF H_2^+ UPON EXPOSURE TO AN INTENSE PULSED PHOTONIC FOCK-STATE", J. PHYS. CHEM A, 113, 7331 (2009).
88	R. GRANOT AND **R. BAER** "A TIGHT-BINDING POTENTIAL FOR HELIUM IN CARBON SYSTEMS", J. CHEM. PHYS. 129, 214102 (2008).
87	E. LIVSHITS AND **R. BAER** "A DENSITY FUNCTIONAL THEORY FOR SYMMETRIC RADICAL CATIONS FROM BONDING TO DISSOCIATION", J. PHYS. CHEM. A,112, 12789 (2008).
86	E. RABANI AND **R. BAER** "DISTRIBUTION OF CARRIER MULTIPLICATION RATES IN CDSE AND INAS NANOCRYSTALS", NANO LETTERS, 8, 4488 (2008).

No.	PUBLICATION
85	R. GRANOT AND **R. BAER** "A SPLINE FOR YOUR SADDLE", J. CHEM. PHYS. 128, 184111 (2008).
84	O. HOD, **R. BAER** AND E. RABANI "MAGNETO-RESISTANCE OF NANOSCALE MOLECULAR DEVICES BASED ON AHARONOV-BOHM INTERFEROMETRY", J. PHYS C, 20, 383201, (2008).
83	**R. BAER** AND E. RABANI "THEORY OF RESONANCE ENERGY TRANSFER INVOLVING NANOCRYSTALS: THE ROLE OF HIGH MULTIPOLES", J. CHEM. PHYS. 128, 184710 (2008).
82	**R. BAER**, "ON THE MAPPING OF TIME-DEPENDENT DENSITIES ONTO POTENTIALS IN QUANTUM MECHANICS", J. CHEM. PHYS. 128, 044103 (2008).
81	Y. KURZWEIL AND **R. BAER**, "ADAPTING APPROXIMATE MEMORY POTENTIALS FOR TIME-DEPENDENT DENSITY FUNCTIONAL THEORY", PHYS. REV. B 77, 085121 (2008).
80	R.JORN, E. LIVSHITS, **R. BAER** AND T. SEIDEMAN, "THE ROLE OF CHARGE LOCALIZATION IN CURRENT-DRIVEN DYNAMICS", ISR. J. CHEM, 47, 99, (2007).
79	E. LIVSHITS AND **R. BAER**, "A WELL-TEMPERED DENSITY FUNCTIONAL THEORY OF ELECTRONS IN MOLECULES", PCCP 9, 2932 (2007).
78	K. LOPATA, D. NEUHAUSER AND **R. BAER**, "CURVE CROSSING AND NEGATIVE REFRACTION IN SIMULATIONS OF NEAR-FIELD COUPLED METALLIC NANOPARTICLE ARRAYS", J. CHEM. PHYS. 127, 154714 (2007)
77	G. J. HALASZ, A. VIBOK, **R. BAER** AND M. BAER, "CONICAL INTERSECTIONS INDUCED BY THE RENNER EFFECT IN POLYATOMIC MOLECULES ", J. PHYS. A 40, F267 (2007).
76	**R. BAER**, K. LOPATA AND D. NEUHAUSER, "PROPERTIES OF PHASE COHERENT ENERGY SHUTTLING ON THE NANOSCALE", J. CHEM. PHYS. 126, 014705 (2007).
75	O. HOD, **R. BAER**, AND E. RABANI, "INELASTIC EFFECTS IN AHARONOV-BOHM MOLECULAR INTERFEROMETERS", PHYS. REV. LETT. 97, 266803 (2006).
74	G. J. HALASZ, A. VIBOK, **R. BAER** AND M. BAER, "D-MATRIX ANALYSIS OF THE RENNER-TELLER EFFECT: AN ACCURATE THREE-STATE DIABATIZATION FOR NH2", J. CHEM. PHYS. 125, 094102 (2006).
73	**R. BAER** E. LIVSHITS AND D. NEUHAUSER, "AVOIDING SELF REPULSION IN DENSITY FUNCTIONAL DESCRIPTION OF BIASED MOLECULAR JUNCTIONS", CHEM. PHYS., 329, 266 (2006).
72	**R. BAER** AND D. NEUHAUSER, "THEORETICAL STUDIES OF MOLECULAR-SCALE NEAR-FIELD ELECTRON DYNAMICS", J. CHEM. PHYS. 125, 074709 (2006).
71	Y. KURZWEIL AND **R. BAER**, "QUANTUM MEMORY EFFECTS ON THE DYNAMICS OF ELECTRONS IN GOLD CLUSTERS", PHYS. REV. B 73, 075413 (2006).
70	E. LIVSHITS AND **R. BAER**, "TIME-DEPENDENT DENSITY-FUNCTIONAL STUDIES OF THE D_2 COULOMB EXPLOSION", J. PHYS. CHEM. 110, 8443 (2006).
69	G. J. HALASZ, A. VIBOK, **R. BAER** AND M. BAER, "RENNER-TELLER NONADIABATIC COUPLING TERMS: AN AB-INITIO STUDY OF THE HNH MOLECULE", J. CHEM. PHYS. 124 081106 (2006).
68	S. JACOBI AND **R. BAER**, "VARIATIONAL GRAND CANONICAL ELECTRONIC STRUCTURE METHOD FOR OPEN SYSTEMS", J. CHEM. PHYS. 123, 044112 (2005).

No.	PUBLICATION
67	D. SHEMESH, **R. BAER**, T. SEIDEMAN AND R. B. GERBER, "PHOTOIONIZATION DYNAMICS OF GLYCINE ADSORBED ON A SILICON CLUSTER: "ON-THE-FLY" SIMULATIONS", J. CHEM. PHYS. 122, 183704 (2005).
66	O. HOD, E. RABANI AND **R. BAER**, "MAGNETO-RESISTANCE OF NANOSCALE MOLECULAR DEVICES", ACC. CHEM. RES. 39, 109 (2006).
65	D. NEUHAUSER AND **R. BAER**, "EFFICIENT LINEAR-RESPONSE METHOD CIRCUMVENTING THE EXCHANGE-CORRELATION KERNEL: THEORY FOR MOLECULAR CONDUCTANCE UNDER FINITE BIAS", J. CHEM. PHYS. 123, 204105 (2005).
64	**R. BAER**, Y. KURZWEIL AND L. S. CEDERBAUM, "TIME-DEPENDENT DENSITY FUNCTIONAL THEORY FOR NON-ADIABATIC PROCESSES", ISR. J. CHEM. 45, 161(2005).
63	O. HOD, **R. BAER**, E. RABANI, "A PARALLEL ELECTROMAGNETIC MOLECULAR LOGIC GATE", J. AM. CHEM. SOC. 127, 1648 (2005).
62	**R. BAER** AND D. NEUHAUSER, "DENSITY FUNCTIONAL THEORY WITH CORRECT LONG-RANGE BEHAVIOR", PHYS. REV. LETT. 94, 043002 (2005).
61	I. RYB AND **R. BAER**, "COMBINATORIAL INVARIANTS AND COVARIANTS AS TOOLS FOR CONICAL INTERSECTIONS", J. CHEM. PHYS. 121, 10370 (2004).
60	O. HOD, E. RABANI AND **R. BAER**, "MAGNETORESISTANCE DEVICES BASED ON SINGLE WALLED CARBON NANOTUBES", J. CHEM. PHYS. 123, 051103 (2005).
59	**R. BAER** AND N. SIAM, "REAL-TIME STUDY OF THE ADIABATIC ENERGY LOSS DURING AN ATOM-METAL CLUSTER COLLISION", J. CHEM. PHYS. 121, 6341 (2004).
58	Y. KURZWEIL AND **R. BAER** "GALILEAN-INVARIANT EXCHANGE-CORRELATION FUNCTIONALS WITH QUANTUM MEMORY", PHYS. REV B 72, 035106 (2005).
57	Y. KURZWEIL AND **R. BAER** "TIME-DEPENDENT EXCHANGE-CORRELATION CURRENT DENSITY FUNCTIONALS WITH MEMORY", J. CHEM. PHYS. 121, 8731 (2004).
56	M. F. HAWTHORNE, J. I. ZINK,J. M. SKELTON, M. J. BAYER, C. LIU, E. LIVSHITS, **R. BAER**, D. NEUHAUSER , "ELECTRICAL OR PHOTOCONTROL OF THE ROTARY MOTION OF A METALLACARBORANE", SCIENCE, 303, 1849 (2004).
55	O. HOD, **R. BAER**, AND E. RABANI, "FEASIBLE NANOMETRIC MAGNETORESISTANCE DEVICES", J. PHYS. CHEM. B, 108, 14807 (2004).
54	Y. B. BAND, S. KALLUSH, AND **R. BAER**, "ROTATIONAL ASPECTS OF SHORT-PULSE POPULATION TRANSFER IN DIATOMIC MOLECULES", CHEM. PHYS. LETT., 23, 392, (2004).
53	**R. BAER**, S. WEISS AND D. NEUHAUSER "ENHANCED ABSORPTION INDUCED BY A METALLIC NANOSHELL", NANOLETTERS, 4, 85 (2004).
52	**R. BAER** AND D. NEUHAUSER "REAL-TIME LINEAR-RESPONSE FOR TIME-DEPENDENT DENSITY-FUNCTIONAL THEORY", J. CHEM. PHYS. 121, 9803 (2004).

No.	PUBLICATION
51	R. COLLEPARDO-GUEVARA, D. WALTER ,D. NEUHAUSER AND **R. BAER**, "A HÜCKEL STUDY OF THE EFFECT OF A MOLECULAR RESONANCE CAVITY ON THE QUANTUM CONDUCTANCE OF AN ALKENE WIRE", CHEM. PHYS. LETT., 393, 367 (2004).
50	**R. BAER**, T. SEIDEMAN, S. ILANI AND D. NEUHAUSER "AB-INITIO STUDY OF THE AC IMPEDANCE OF A MOLECULAR JUNCTION", J. CHEM. PHYS. 120, 3387 (2004).
49	S. JACOBI AND **R. BAER**, "THE WELL-TEMPERED AUXILIARY-FIELD MONTE CARLO", J. CHEM. PHYS. 120, 43 (2003).
48	W.-Z. LIANG, C. SARAVANAN, Y. SHAO, **R. BAER**, A. T. BELL AND M. HEAD-GORDON, "IMPROVED FERMI OPERATOR EXPANSION METHODS FOR FAST ELECTRONIC STRUCTURE CALCULATIONS", J. CHEM. PHYS. 119 4117 (2003).
47	**R. BAER**, D. J. KOURI, M. BAER AND D. K. HOFFMAN "GENERAL BORN-OPPENHEIMER-HUANG APPROACH TO SYSTEMS OF ELECTRONS AND NUCLEI", J. CHEM. PHYS., 119, 6998 (2003).
46	C. SARAVANAN, Y. SHAO, **R. BAER**, P. N. ROSS, M. HEAD-GORDON, "SPARSE MATRIX MULTIPLICATIONS FOR LINEAR SCALING ELECTRONIC STRUCTURE CALCULATIONS IN AN ATOM-CENTERED BASIS SETS USING MULTI-ATOM BLOCKS", J. OF COMP. CHEM., 24, 618 (2003).
45	R.BAER, D. NEUHAUSER, P.R. ZDANSKA AND N. MOISEYEV, "IONIZATION AND HIGH-HARMONIC GENERATION IN ALIGNED BENZENE BY INTENSE CIRCULARLY POLARIZED LIGHT", PHYS REV A 68, 043406 (2003).
44	S. M. ANDERSON, D. NEUHAUSER, AND **R. BAER**, "TRAJECTORY DEPENDENT CELLU-LARIZED FROZEN GAUSSIANS (TDCFG), A NEW APPROACH FOR SEMI-CLASSICAL DYNAMICS: THEORY AND APPLICATION TO HE-NAPHTHALENE EIGENVALUES", J. CHEM. PHYS. 118, 9103 (2003).
43	D. NEUHAUSER AND **R. BAER**, "A TWO-GRID FORMALISM FOR THE MAXWELL EQUATION", J. THEO. AND COMP. CHEM. 2, 537 (2003).
42	W-Z LIANG, **R. BAER**, C. SARAVANAN, Y. SHAO, A. T. BELL, M. HEAD-GORDON, "FAST METHODS FOR RESUMMING MATRIX POLYNOMIALS AND CHEBYSHEV MATRIX POLYNOMIALS", J. COMPUT. PHYS. 194, 575 (2004).
41	D. NEUHAUSER, **R. BAER** AND R. KOSLOFF, "QUANTUM SOLITON DYNAMICS IN VIBRATIONAL CHAINS: COMPARISON OF FULLY CORRELATED, MEAN FIELD, AND CLASSICAL DYNAMICS" J. CHEM. PHYS. 118, 5729 (2003).
40	**R. BAER** AND D. NEUHAUSER, "MANY-BODY SCATTERING FORMALISM OF QUANTUM MOLECULAR CONDUCTANCE", CHEM. PHYS. LETT. 374, 459 (2003).
39	C. LIU, D. WALTER, D. NEUHAUSER AND **R. BAER**,"MOLECULAR RECOGNITION AND CONDUCTANCE IN CROWN ETHER", J. AM. CHEM. SOC. 125 (46), 13936 (2003).
38	D. WALTER, D. NEUHAUSER AND **R. BAER**, "QUANTUM INTERFERENCE IN POLYCYCLIC AROMATIC HYDROCARBON BASED MOLECULAR DYNAMICS", PHYS. CHEM., 299, 139 (2002).
37	A. LUCHOW, D. NEUHAUSER, J. KA, **R. BAER**, J. CHEN, V. A. MANDELSHTAM, "COMPUTING ENERGY LEVELS BY INVERSION OF IMAGINARY-TIME CROSS-CORRELATION FUNCTIONS", J. PHYS. CHEM. A 107, 7175 (2003).

No.	PUBLICATION
36.	O. HOD, E. RABANI AND **R. BAER**, "CARBON NANOTUBE CLOSED-RING STRUCTURES", PHYS. REV. B 67, 195408, (2003).
35.	H. SZICHMAN AND **R. BAER**, "A FIVE DIMENSIONAL QUANTUM MECHANICAL STUDY OF THE REACTION H+CH4→H2+CH3", J. CHEM. PHYS. 117, 7614 (2002).
34.	**R. BAER**, "BORN-OPPENHEIMER INVARIANTS ALONG NUCLEAR PATHS", J. CHEM. PHYS. 117, 7405 (2002).
33.	**R. BAER**, "NONADIABATIC COUPLINGS BY TIME-DEPENDENT DENSITY FUNCTIONAL THEORY", CHEM. PHYS. LETT., 364, 75 (2002).
32.	**R. BAER** AND D. NEUHAUSER, "ANTI-COHERENCE-BASED MOLECULAR ELECTRONICS: XOR-GATE RESPONSE", CHEM. PHYS. 281, 353 (2002).
31.	**R. BAER** AND D. NEUHAUSER, "AB INITIO CONDUCTANCE OF A MOLECULAR WIRE", INT. J. OF QUANT. CHEM. 91, 524(2002).
30.	**R. BAER** AND D. NEUHAUSER, "PHASE COHERENT ELECTRONICS: A MOLECULAR SWITCH BASED ON QUANTUM INTERFERENCE", J. AM. CHEM. SOC. 124(16) 4200 (2002).
29.	**R. BAER** AND D. NEUHAUSER, "SHIFTED CONTOUR AUXILIARY FIELD MONTE CARLO", IN: RECENT ADVANCES IN QUANTUM MONTE CARLO METHODS II, EDITORS: W.A. LESTER JR., S. ROTHSTEIN AND S. TANAKA, WORLD SCIENTIFIC (2002).
28.	**R. BAER**, "AB INITIO COMPUTATION OF SINGLET-TRIPLET MOLECULAR ENERGY DIFFERENCES USING AUXILIARY FIELD MONTE CARLO", CHEM. PHYS. LETT. 343 535 (2001).
27.	S. ADHIKARI AND **R. BAER**, "AUGMENTED LAGRANGIAN METHOD FOR ORDER-N ELECTRONIC STRUCTURE", J. CHEM. PHYS. 115, 11 (2001).
26.	**R. BAER** AND R. GOULD, "A METHOD FOR AB INITIO NONLINEAR ELECTRON DENSITY EVOLUTION", J. CHEM. PHYS. 114, 3385 (2001).
25.	**R. BAER** "NONLINEAR EVOLUTION OF ELECTRONIC DENSITY IN MOLECULES", IN: MULTISCALE COMPUTATIONAL METHODS IN CHEMISTRY AND PHYSICS, EDS: A. BRANDT, J. BERNHOLC AND K. BINDER, VOLUME 177 OF NATO SCIENCE SERIES, (IOS PRESS, AMSTERDAM 2001).
24.	**R. BAER**, "ACCURATE AND EFFICIENT EVOLUTION OF NONLINEAR SCHRODINGER EQUATIONS", PHYS. REV A , 62, 063810 (2000).
23.	**R. BAER**, "AB-INITIO MOLECULAR DEFORMATION BARRIERS USING AUXILIARY-FIELD QUANTUM MONTE CARLO WITH APPLICATION TO THE INVERSION BARRIER OF WATER", CHEM. PHYS. LETT. 324, 101 (2000).
22.	**R. BAER**, "AB-INITIO COMPUTATION OF FORCES AND MOLECULAR SPECTROSCOPIC CONSTANTS USING PLANEWAVE BASED AUXILIARY FIELD MONTE CARLO WITH APPLICATION TO N2", J. CHEM. PHYS. 113, 473 (2000).
21.	D. BARASH, A. E. OREL AND **R. BAER**, "A COMMENT ON THE STABILIZATION OF A ONE-DIMENSIONAL SHORT-RANGE MODEL ATOM IN INTENSE LASER FIELDS", J. PHYS. B 33, 1279 (2000).

No.	PUBLICATION
20.	**R. BAER** AND D. NEUHAUSER, "MOLECULAR ELECTRONIC STRUCTURE USING AUXILIARY FIELD MONTE CARLO, PLANE WAVES AND PSEUDOPOTENTIALS" J. CHEM. PHYS. 112, 1679 (2000).
19.	D. BARASH, A. OREL AND **R. BAER** "LASER INDUCED RESONANCE STATES AS A CAUSE FOR DYNAMIC SUPPRESSION OF IONIZATION IN HIGH FREQUENCY SHORT PULSES" PHY. REV. A, 61, 13402 (2000).
18.	**R. BAER** AND M. HEAD-GORDON, "ELECTRONIC STRUCTURE OF LARGE SYSTEMS: COPING WITH SMALL GAPS USING THE ENERGY RENORMALIZATION GROUP METHOD" J. CHEM. PHYS. 109, 10159 (1998).
17.	**R. BAER** AND M. HEAD-GORDON, "ENERGY RENORMALIZATION GROUP METHOD FOR ELECTRONIC STRUCTURE OF LARGE SYSTEMS" PHYS. REV B. 58, 15296 (1998).
16.	**R. BAER**, M. HEAD-GORDON AND D. NEUHAUSER, "SHIFTED-CONTOUR AUXILIARY FIELD MONTE CARLO FOR AB INITIO ELECTRONIC STRUCTURE: STRADDLING THE SIGN PROBLEM" J. CHEM. PHYS.109, 6219 (1998).
15.	**R. BAER**, Y. ZEIRI AND R. KOSLOFF, "QUANTUM DIFFUSION OF HYDROGEN AND DEUTERIUM ON NICKEL (100)", SURF. SCI., 411, L783 (1998).
14.	**R. BAER** AND M. HEAD-GORDON, "CHEBYSHEV EXPANSION METHODS IN CALCULATIONS OF ELECTRONIC STRUCTURE OF LARGE MOLECULES" J. CHEM. PHYS. 107, 10003 (1997).
13.	**R. BAER** AND M. HEAD-GORDON, "ON THE SPARSITY OF THE ONE ELECTRON DENSITY MATRIX AND LINEAR SCALING CALCULATIONS" PHYS. REV. LETT. 79, 3962 (1997).
12.	D. M. CHARUTZ, **R. BAER** AND M. BAER, "A STUDY OF DEGENERATE VIBRONIC COUPLING EFFECTS ON SCATTERING PROCESSES: ARE RESONANCES AFFECTED BY DEGENERATE VIBRONIC COUPLING?" CHEM. PHYS. LETT, 265, 629 (1997).
11.	**R. BAER**, Y. ZEIRI AND R. KOSLOFF, "HYDROGEN TRANSPORT IN NICKEL (111)" PHYS. REV. B. 55, 10952 (1997).
10.	**R. BAER** AND R. KOSLOFF, "QUANTUM DISSIPATIVE DYNAMICS OF ADSORBATES NEAR METAL SURFACES: A SURROGATE HAMILTONIAN THEORY APPLIED TO HYDROGEN ON NICKEL", J. CHEM. PHYS. 106, 8862 (1997).
9.	**R. BAER**, D. CHARUTZ, R. KOSLOFF AND M. BAER, "THE VALIDITY OF ADIABATIC SINGLE-SURFACE APPROXIMATIONS WITHIN AN EXTENDED JAHN-TELLER MODEL", J. CHEM. PHYS., 105, 9141 (1996).
8.	**R. BAER**, Y. ZEIRI AND R. KOSLOFF, "THE INFLUENCE OF DIMENSIONALITY ON DEEP TUNNELING RATES: A STUDY BASED ON THE HYDROGEN NICKEL SYSTEM", PHYS. REV. B, (RAP. COMM.) 54, R5287 (1996).
7.	O. CITRI, **R. BAER** AND R. KOSLOFF, "THE ROLE OF NON-ADIABATIC MECHANISMS IN THE DISSOCIATION DYNAMICS OF O2 ON SILVER SURFACES", SURF. SCI. 351,24 (1996).
6.	E. FATTAL, **R. BAER** AND R. KOSLOFF, "A PHASE SPACE APPROACH FOR OPTIMIZING GRID REPRESENTATION: THE MAPPED FOURIER METHOD", PHYS. REV. E, 53, 1217 (1996).
5.	G. KATZ, **R. BAER** AND R. KOSLOFF, "A NEW METHOD FOR NUMERICAL FLUX CALCULATIONS IN MOLECULAR DYNAMICS", CHEM. PHYS. LETT. 239, 230 (1995).

No.	PUBLICATION
4.	**R. BAER** AND R. KOSLOFF, "INVERSION OF ULTRASHORT PUMP-PROBE SPECTROSCOPIC DATA", J. PHYS. CHEM., 99, 2534-2545 (1995).
3.	P.SAALFRANK, **R. BAER** AND R. KOSLOFF, "DENSITY MATRIX DESCRIPTION OF LASER-INDUCED, HOT ELECTRON MEDIATED PHOTODESORPTION OF NO FROM PT(111)" CHEM PHYS. LETT. 230, 463 (1994).
2.	**R. BAER** AND R. KOSLOFF, "OBTAINING THE EXCITED-STATE POTENTIAL BY INVERSION OF PHOTODISSOCIATION ABSORPTION SPECTRA", CHEM. PHYS. LETT., 200, 183 (1992).
1.	R. KOSLOFF AND **R. BAER**, "IMPULSIVE ITERATIVE INVERSION", IN MODE SELECTIVE CHEMISTRY JERUSALEM SYMPOSIA ON QUANTUM CHEMISTRY AND BIOCHEMISTRY, VOL. 24, EDS. J. JORTNER, R. D. LEVINE AND B. PULLMAN (KLUWER, DORDECHT, 1991) P. 345.

Invited Talks (2004-today)

No.	Year	Month	Dates	Conference/Workshop	Place	Presentation Title
88	2018	8	28-31	CECAM Workshop on TDDFT	Benasque Spain	
87	2018	4	9-12	CECAM Workshop Strongly Correlated Electrons	Tel Aviv	
86	2018	3	18-22	Adventures in Density Functional Theory	New Orleans (ACS meeting)	
85	2017	11	8-10	Nimrod Moiseyev Fest meeting	Technion	
84	2017	8	27-31	WATOC meeting	Munich Germany	Stochastic approaches to electronic structure
83	2017	6	20-24	New Frontiers in Electron Correlation	Telluride	Stochastic approaches to electronic structure
82	2017	5	19	Fundamentals of Density Functional Theory: A Celebration of the Works of Mel Levy	CUNY New York	Optimally-Tuned Generalized Kohn Sham Theory
81	2016	9	26-30	CTTC2016	Peru	Last moment cancel (Family)
80	2016	9	19-23	The Molecular Electronic Structure (MES)	Buenos Aires, Argentina	Stochastic approaches to perturbation theory
79	2016	7	20	Kavli ENSI Faculty talk	UC Berkeley, California	Stochastic approaches to electronic structure
78	2016	7	6	Dept. Visit UC Merced	Merced California	Stochastic approaches to electronic structure
77	2016	6	4	Quantum Day	Technion	Stochastic approaches to perturbation theory
76	2016	3	25-27	3 Departmental visits: Univ Michigan at Ann Arbor, Wayne Univ. and Michigan State	Michigan USA	Stochastic approaches to perturbation theory
75	2016	6	1-5	LUEST Meeting	Telluride	Stochastic approaches to perturbation theory
74	2016	5	2	Departmental visit	UC Irvine	Charge-carrier localization in extended systems
73	2015	12	30	Phys Chem Seminar – UC Berkeley	UC Berkeley	Charge-carrier localization in extended systems
72	2015	11-12	30-4	CECAM WORKSHOP on Open Quantum Systems	Hong Kong	Had to cancel last minute. Family reasons.
71	2015	9	20-24	STC 2015	Pottsdam, Germany	Charge-carrier localization in extended systems
70	2015	4	21-25	CECAM Meeting: Stochastic Wavefunction Methods in Quantum Chemistry, Electronic Structure Theory and Condensed Matter Phys-	EPFL Lausanne	Stochastic methods for DFT on very large systems

No.	Year	Month	Dates	Conference/Workshop	Place	Presentation Title
				ics		
69	2015	4	7-10	CECAM Meeting: Charge Transfer Modeling in Chemistry: new methods and solutions for a long-standing problem	Paris France	Stochastic Electronic Structure for Very Large Molecular Systems
68	2015	3	15	German Physics Society Meeting: Symposium on Frontiers of Electronic Structure Theory - Many-body effects on the nano-scale	Berlin	Stochastic density functional and GW theories scaling linearly with system size
67	2015	1	7-11	9th International Conference on Computational Phyiscs (ICCP9)	Singaopore	Stochastic density functional and GW theories scaling linearly with system size
66	2014	11	13	Colloquium Speaker	Technion	Quasiparticles in molecular systems
65	2014	10	9	University of California, San Diego	Sand Diego, California, USA	Stochastic wave functions for large scale electronic structure
64	2014	4	9-11	PQI2014: Quantum Technologies	Pittsburgh, USA	Stochastic methods for gentle scaling of electronic structure methods with acronyms we love and trust
63	2014	3	15-19	ACS Meeting	Dallas Texas	Stochastic methods for gentle scaling of electronic structure methods with acronyms we love and trust
62	2014	2	16 - 24	Sanibel Synposium	St. Simons Island, Georgia, USA	Self-averaging stochastic Kohn-Sham density functional theory
61	2014	1	14-17	6th Workshop on Time-Dependent Density-Functional Theory: Prospects and Applications	Benasque, Spain	Stochastic methods for gentle scaling of electronic structure methods with acronyms we love and trust (DFT, MP2, RPA, GW)
61	2014	1	9-11	International workshop on computational physics and materials science ("Total energy and force methods")	Lausanne, Switzerland	Self-averaging stochastic Kohn-Sham density functional theory
60	2013	11	28-	Quantum Dynamics in Molecular and Nano-Materials: Mechanisms and Functionality	Tel Aviv University	Stochastic Approaches to Electronic Structure
59	2013	8	11-16	Gordon Research Conference on Time Dependent Density Functional Theory	University of New England, Biddeford, Maine, USA	TBA
58	2013	4	23-26	TDDFT-Nantes 2013	University of Nantes, France	Orbital energies in density functional theory
57	2012	9	10-14	From Density Functional	Bayreuth, GER-	Orbital energies and energy

No.	Year	Month	Dates	Conference/Workshop	Place	Presentation Title
				Theory principles to material properties	MANY	curvature in density functional theory
56	2012	8	19-23	Fall 2012 National Meeting of the American Chemical Society	Philadelphia Convention Center, Pennsylvania, USA	A new first-principles approach to Density Functional Theory: "Tuned" range separated hybrids. Why they work and when are they needed
55	2012	7	4-6	CECAM: Theoretical Challenges in Electronic Structure of Clusters and Nanoparticles	CECAM-HQ-EPFL, Lausanne, SWITZERLAND	The "Tuned" Range Separated Hybrid in Density Functional Theory: Why and How They Work
54	2012	7	16-20	Molecular Electronics in Jerusalem	Inst of Advanced Studies, Jerusalem, ISRAEL	A First Principles Density Functional Approach that should be usefed for transport in weakly coupled molecular junctions
53	2012	5	14-15	The first French - israeli inter-academy meeting in chemistry	The Israel Academy of Sciences and Humanities, Jerusalem, ISRAEL	A New First-Principles Approach to Density Functional Theory: “Tuned” Range Separated Hybrids. Why they work and when are they indispensable
52	2012	4	30-4	Kathmandu Workshop on Theoretical Chemistry	Radisson Hotel, Kathmandu, NEPAL	Dogmatic and Pragmatic Spirits in Density Functional Theory
51	2012	2	7-8	77th Annual Meeting of the Israel Chemical Society	Kfar Hamaccabia, ISRAEL	Density Functional Approach For Molecular Junctions: Charge-Transfer And Conductance In A Non-Mechanical Molecular Switch
50	2011	11	9	Invited Seminar	Bar Ilan University	Density functional approach for molecular electronics and photovoltaics
49	2011	9	19-23	CECAM: Perspectives and Challenges of Many Particle Methods	Univ. of Bremen GERMANY	Tuned Range Separated Hybrids: Fundamental Gaps and Excitation Energies of finite systems
48	2011	9	2-8	VIIth Congress of the International Society for Theoretical Chemical Physics	Waseda University, Tokyo, JAPAN	A first-principles density functional approach for charge transfer & transport
47	2011	8	14-19	Gordon Research Conference on Time Dependent Density Functional Theory	University of New England, Biddeford, Maine, USA	Orbital energies in density functional theory (originally invited to chair a session, but due to cancellation, invited to speak. Elected to be Chair of “2015 GRC on TDDFT”)
46	2011	6	20-24	CECAM: How to Speed Up Progress and Reduce Empiricism in Density Functional Theory	ACAM, Dublin, IRELAND	A first-principles density functional approach for charge transfer & transport

No.	Year	Month	Dates	Conference/Workshop	Place	Presentation Title
45	2011	2	9	Invited Seminar	Max Planck Institute for Microstructure Physics, Halle	Tuned Range Separated Hybrids: Fundamental Gaps and Excitation Energies of finite systems
44	2011	2	7	Invited Seminar	Dept of Physics, Bayreuth University	Tuned Range Separated Hybrids: Fundamental Gaps and Excitation Energies of finite systems
43	2010	12	15-19	Current Trends in Condensed Matter Physics	National Inst of Science Education and Research, Bubanasewar, INDIA	Molecular Conical Intersections and Density Functional Theory
42	2010	11	8	Invited Seminar	Ben Gurion University	A density functional approach for charge transfer and charge transport
41	2010	9	28	Invited Seminar	Helenic Academy of Sciences Athens	A density functional approach for charge transfer and charge transport
40	2010	5	12-15	CECAM workshop: Quantum transport and dynamics in materials and biosystems: From molecular mechanisms to mesoscopic functionality	ACAM, Dublin, IRELAND	A density functional approach for charge transfer and charge transport
39	2010	2	7-8	75th Israel Chemical Society National meeting	Kfar Hamaccabiah	Orbital energies as quasi-particle energies in density functional theory
38	2010	1	10-15	4th Benasque Time-Dependent Density-Functional Theory: Prospects and Applications	Benasque, Spain	Pragmatic and Dogmatic Spirits in Time-Dependent Density Functional Theory
37	2010	1	27	Invited Seminar	ARL Aberdeen USA	Tuned Range Separated Hybrids for DFT
36	2010	1	25-26	75th Israel Chemical Society National meeting	David Intercontinental	TUNED RANGE-SEPERATED HYBRIDS FOR DENSITY FUNCTIONAL THEORY
35	2009	7	6	Invited Seminar	Physics Dept, Ludwig Maxemillian University Munich	Density functional theories that respect the quantum nature of charge + Carrier multiplication in Nanocrystals
34	2009	4	2-8	Second International Symposium and Workshop on Correlated Electrons in Matter	Park Vista Hotel, Gatlinburg, TN, USA	Dogmatic and Pragmatic Spirits in Time-Dependent Density Functional Theory
33	2009	1	11-16	IMA Thematic Theoretical Chemistry workshop	Institute of Mathematics and Applications, University of Minnesota	Dogmatic and Pragmatic Spirits in Time-Dependent Density Functional Theory
32	2008	21	5	Invited Seminar	Ben Gurion Uni-	Dogmatic and Pragmatic Spirits

No.	Year	Month	Dates	Conference/Workshop	Place	Presentation Title
					versity	in Time-Dependent Density Functional Theory
31	2008	9	29	Invited Seminar	Dept of Mathematics San Diego State university	Dogmatic and Pragmatic Spirits in Time-Dependent Density Functional Theory
30	2008	9	8	Invited Seminar	Dept. of Chemistry, University of Southern California	Dogmatic and Pragmatic Spirits in Time-Dependent Density Functional Theory
29	2008	9	10-15	3rd Benasque Workshop on TDDFT	Bensque Science Center, Spain	Dogmatic and Pragmatic Spirits in Time-Dependent Density Functional Theory
28	2008	5	9-13	Workshop on range-separated hybrids (RSH),	University of Paris Jussieu, France	A DFT for symmetric radical cations: from bonding to dissociation
27	2008	4	16	Invited Seminar	University of Cyprus	Dogmatic and Pragmatic Spirits in Time-Dependent Density Functional Theory
26	2008	1	10	Invited Seminar	School of Chemistry, TAU	Pragmatic and dogmatic spirits in theory of metal nanoparticle excitations
25	2008	1	10	Physical Chemistry Symposium	School of Chemistry, TAU	Dogmatic and Pragmatic Spirits in Time-Dependent Density Functional Theory
24	2007	12	16-21	Gentner Symposium on TDDFT	Queen of Sheba Hotel, Eilat Israel	Range Separated Hybrids
23	2007	9		Safed Summer School on DFT	Safed Israel	Real time TDDFT and applications
22	2007	7	15-20	Gordon Research Conference on Time Dependent Density Functional Theory	Colby College, Waterville, ME	A search for improved TDDFT functionals
21	2007	3	20	Invited Seminar	Holon Inst of technology	Time-dependent density functional theory for near-field - electron dynamics
20	2007	2	6-7	72nd Israel Chemical Society National meeting	Hilton Tel Aviv	A well-tempered density functional theory
19	2006	12	4-8	CECAM workshop: Quantum transport and nonadiabatic electron evolution from first principles approaches	CECAM 46, Lyon, France	Density Functional Theory and molecular junctions
18	2006	12	20	Invited Seminar	Faculty of Chemistry, Technion	Time-dependent density functional theory for near-field - electron dynamics
17	2006	10	18	Invited Seminar	Dept of Chemistry, University of Regensburg, Germany	Towards time-dependent density functional theory for near-field - electron dynamics

No.	Year	Month	Dates	Conference/Workshop	Place	Presentation Title
16	2006	9	6-11	2nd Benasque Workshop on TDDFT	Bensque Science Center, Spain	Towards time-dependent density functional theory for near-field - electron dynamics
15	2006	5	31	Invited Seminar	Dept of Chemistry, Caltech	Towards time-dependent density functional theory for near-field - electron dynamics
14	2006	4	28	Invited Seminar	Dept of Chemistry, University of Iowa, USA	Towards time-dependent density functional theory for near-field - electron dynamics
13	2006	3	26-3	47th Sanibel Symposium	St. Simons Island Georgia	Towards time-dependent density functional theory for near-field - electron dynamics
12	2006	3	29	ACS National Spring Meeting	Atlanta Georgia	Towards time-dependent density functional theory for near-field - electron dynamics
11	2006	2	17	Invited Seminar	Dept of Chemistry, University of Michigan Ann Arbor	Theoretical studies of near-field - electron dynamics on small length scales
10	2005	11	28-2	International Workshop on ”Atomic Physics”	Max-Planck-Institut für Physik komplexer Systeme, Desden, Germany	Time dependent density functional theory beyond adiabatic approximation: New approaches and applications
9	2005	5	4	Invited Seminar	Ben Gurion University	3 Tutorial talks on TDDFT
8	2005	3	21	APS Spring National Meeting	Los Angeles Convention center	Advances in density functional description of molecular junctions
7	2004	9	3	Invited Seminar	Dept. of Physics, University of Washington, Seattle	Real-time electron dynamics in molecules and clusters
6	2004	9	7-12	1st Benasque Workshop on TDDFT	Bensque Science Center, Spain	Real-time electron dynamics in molecules and clusters
5	2004	8	1-8	Non adiabatic dynamics	Telluride Science Research Center	Real-time electron dynamics in molecules and clusters
4	2004	7	11-16	Gordon Research Conference on Atomic & Molecular Interactions	Colby-Sawyer College, New London NH	Real-time electron dynamics in molecules and clusters
3	2004	5	13-17	Workshop on nonadiabatic dynamics	Ein Gedi	TDDFT in real time: a general approach to electronic processes
2	2004	4	3	Invited Seminar	Ben Gurion University	Advances in the theory of molecular electronics
1	2004	4	29	Invited Seminar	School of Chemistry, TAU	Ab initio studies of electron dynamics in molecules and clusters