Ivan Duchemin

List of Publications by Year in Descending Order

72 papers	2,387 citations	31 h-index	47 g-index
79 ext. papers	2,725 ext. citations	5.7 avg, IF	5.58 L-index

#	Paper	IF	Citations
72	Modeling of the Bandgap Distribution in Bi-Axially Strained Germanium Crossbeam for Laser Applications. *IEEE Photonics Journal*, **2022**, 14, 1-4	1.8	0
71	Cubic-Scaling All-Electron Calculations with a Separable Density-Fitting Space-Time Approach. *Journal of Chemical Theory and Computation*, **2021**, 17, 2383-2393	6.4	17
70	Photoluminescent properties of the carbon-dimer defect in hexagonal boron-nitride: A many-body finite-size cluster approach. *Physical Review Materials*, **2021**, 5,	3.2	2
69	Robust Analytic-Continuation Approach to Many-Body Calculations. *Journal of Chemical Theory and Computation*, **2020**, 16, 1742-1756	6.4	23
68	Optical properties of graphene quantum dots: the role of chiral symmetry. *2D Materials*, **2020**, 7, 025041	5.9	2
67	Pros and Cons of the Bethe-Salpeter Formalism for Ground-State Energies. *Journal of Physical Chemistry Letters*, **2020**, 11, 3536-3545	6.4	15
66	Ground-state correlation energy of beryllium dimer by the Bethe-Salpeter equation. *SciPost Physics*, **2020**, 8,	6.1	8
65	The Bethe-Salpeter Equation Formalism: From Physics to Chemistry. *Journal of Physical Chemistry Letters*, **2020**, 11, 7371-7382	6.4	38
64	Separable resolution-of-the-identity with all-electron Gaussian bases: Application to cubic-scaling RPA. *Journal of Chemical Physics*, **2019**, 150, 174120	3.9	23
63	Host dependence of the electron affinity of molecular dopants. *Materials Horizons*, **2019**, 6, 107-114	14.4	44
62	The Bethe-Salpeter formalism with polarisable continuum embedding: reconciling linear-response and state-specific features. *Chemical Science*, **2018**, 9, 4430-4443	9.4	37
61	Accurate description of charged excitations in molecular solids from embedded many-body perturbation theory. *Physical Review B*, **2018**, 97,	3.3	34
60	The Bethe-Salpeter equation in chemistry: relations with TD-DFT, applications and challenges. *Chemical Society Reviews*, **2018**, 47, 1022-1043	58.5	110
59	Bethe-Salpeter study of cationic dyes: Comparisons with ADC(2) and TD-DFT. *Journal of Chemical Physics*, **2017**, 146, 034301	3.9	18
58	Benchmark of Bethe-Salpeter for Triplet Excited-States. *Journal of Chemical Theory and Computation*, **2017**, 13, 767-783	6.4	51
57	Hybrid and Constrained Resolution-of-Identity Techniques for Coulomb Integrals. *Journal of Chemical Theory and Computation*, **2017**, 13, 1199-1208	6.4	15
56	A Strategy to Suppress Phonon Transport in Molecular Junctions Using Stacked Systems. *Journal of Physical Chemistry C*, **2017**, 121, 7175-7182	3.8	38

55	Modeling the Photochrome-TiO Interface with Bethe-Salpeter and Time-Dependent Density Functional Theory Methods. *Journal of Physical Chemistry Letters*, **2017**, 8, 936-940	6.4	14
54	Is the Bethe-Salpeter Formalism Accurate for Excitation Energies? Comparisons with TD-DFT, CASPT2, and EOM-CCSD. *Journal of Physical Chemistry Letters*, **2017**, 8, 1524-1529	6.4	61
53	Helium Atom Excitations by the GW and Bethe-Salpeter Many-Body Formalism. *Physical Review Letters*, **2017**, 118, 163001	7.4	16
52	Calculations of n-π* Transition Energies: Comparisons Between TD-DFT, ADC, CC, CASPT2, and BSE/GW Descriptions. *Journal of Physical Chemistry A*, **2017**, 121, 6122-6134	2.8	17
51	Correlated electron-hole mechanism for molecular doping in organic semiconductors. *Physical Review Materials*, **2017**, 1,	3.2	31
50	Assessment of the Accuracy of the Bethe-Salpeter (BSE/GW) Oscillator Strengths. *Journal of Chemical Theory and Computation*, **2016**, 12, 3969-81	6.4	34
49	Combining the Many-Body GW Formalism with Classical Polarizable Models: Insights on the Electronic Structure of Molecular Solids. *Journal of Physical Chemistry Letters*, **2016**, 7, 2814-20	6.4	59
48	Assessment of the convergence of partially self-consistent BSE/GW calculations. *Molecular Physics*, **2016**, 114, 957-967	1.7	16
47	Study of the light emission in Ge layers and strained membranes on Si substrates. *Thin Solid Films*, **2016**, 613, 64-67	2.2	14
46	GW and Bethe-Salpeter study of small water clusters. *Journal of Chemical Physics*, **2016**, 144, 034109	3.9	31
45	Accurate strain measurements in highly strained Ge microbridges. *Applied Physics Letters*, **2016**, 108, 241902	3.4	26
44	Combining the GW formalism with the polarizable continuum model: A state-specific non-equilibrium approach. *Journal of Chemical Physics*, **2016**, 144, 164106	3.9	30
43	Revealing the band structure of InSb nanowires by high-field magnetotransport in the quasiballistic regime. *Physical Review B*, **2016**, 94,	3.3	2
42	Germanium under High Tensile Stress: Nonlinear Dependence of Direct Band Gap vs Strain. *ACS Photonics*, **2016**, 3, 1907-1911	6.3	39
41	First Principles Calculations of Charge Transfer Excitations in Polymer–Fullerene Complexes: Influence of Excess Energy. *Advanced Functional Materials*, **2015**, 25, 1972-1984	15.6	50
40	Benchmarking the Bethe-Salpeter Formalism on a Standard Organic Molecular Set. *Journal of Chemical Theory and Computation*, **2015**, 11, 3290-304	6.4	145
39	Quantum dot made in metal oxide silicon-nanowire field effect transistor working at room temperature. *Nano Letters*, **2015**, 15, 2958-64	11.5	24
38	0-0 Energies Using Hybrid Schemes: Benchmarks of TD-DFT, CIS(D), ADC(2), CC2, and BSE/GW formalisms for 80 Real-Life Compounds. *Journal of Chemical Theory and Computation*, **2015**, 11, 5340-59	6.4	166

37	Remote surface roughness scattering in fully depleted silicon-on-insulator devices with high-/SiO2 gate stacks. *Applied Physics Letters*, **2015**, 106, 023508	3.4	3
36	Mechanical Tuning of Thermal Transport in a Molecular Junction. *Journal of Physical Chemistry C*, **2015**, 119, 24636-24642	3.8	44
35	Non-linear model of electronic band structure to highly tensile-strained Germanium **2015**,		1
34	Exploring approximations to the GW self-energy ionic gradients. *Physical Review B*, **2015**, 91,	3.3	25
33	Phonon-limited carrier mobility and resistivity from carbon nanotubes to graphene. *Physical Review B*, **2015**, 92,	3.3	11
32	1.9% bi-axial tensile strain in thick germanium suspended membranes fabricated in optical germanium-on-insulator substrates for laser applications. *Applied Physics Letters*, **2015**, 107, 191904	3.4	62
31	Does Excess Energy Assist Photogeneration in an Organic Low-Bandgap Solar Cell?. *Advanced Functional Materials*, **2015**, 25, 1287-1295	15.6	30
30	Excited states properties of organic molecules: from density functional theory to the GW and Bethe-Salpeter Green function formalisms. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2014**, 372, 20130271	3	81
29	Quantum Modeling of the Carrier Mobility in FDSOI Devices. *IEEE Transactions on Electron Devices*, **2014**, 61, 3096-3102	2.9	20
28	Benchmark Many-Body GW and Bethe-Salpeter Calculations for Small Transition Metal Molecules. *Journal of Chemical Theory and Computation*, **2014**, 10, 3934-43	6.4	87
27	Quantum calculations of the carrier mobility: Methodology, Matthiessen rule, and comparison with semi-classical approaches. *Journal of Applied Physics*, **2014**, 115, 054512	2.5	38
26	Combining the Bethe-Salpeter Formalism with Time-Dependent DFT Excited-State Forces to Describe Optical Signatures: NBO Fluoroborates as Working Examples. *Journal of Chemical Theory and Computation*, **2014**, 10, 4548-56	6.4	30
25	Few-electron edge-state quantum dots in a silicon nanowire field-effect transistor. *Nano Letters*, **2014**, 14, 2094-8	11.5	54
24	Fast and Accurate Electronic Excitations in Cyanines with the Many-Body Bethe-Salpeter Approach. *Journal of Chemical Theory and Computation*, **2014**, 10, 1212-8	6.4	73
23	Study of the piezoresistive properties of NMOS and PMOS -gate SOI nanowire transistors: Scalability effects and high stress level **2014**,		5
22	Magnetotransport subband spectroscopy in InAs nanowires. *Physical Review Letters*, **2014**, 112, 076801	7.4	14
21	Accurate complex scaling of three dimensional numerical potentials. *Journal of Chemical Physics*, **2013**, 138, 204111	3.9	5
20	Resonant hot charge-transfer excitations in fullerene-porphyrin complexes: Many-body Bethe-Salpeter study. *Physical Review B*, **2013**, 87,	3.3	43

19	Many-body Green function GW and Bethe-Salpeter study of the optical excitations in a paradigmatic model dipeptide. *Journal of Chemical Physics*, **2013**, 139, 194308	3.9	44
18	Multi-scale strategy for high-k/metal-gate UTBB-FDSOI devices modeling with emphasis on back bias impact on mobility. *Journal of Computational Electronics*, **2013**, 12, 675-684	1.8	6
17	Efficient Computation of Hartree-Fock Exchange Using Recursive Subspace Bisection. *Journal of Chemical Theory and Computation*, **2013**, 9, 582-7	6.4	42
16	Mobility in high-K metal gate UTBB-FDSOI devices: From NEGF to TCAD perspectives **2013**,		3
15	Metallic behaviour in SOI quantum wells with strong intervalley scattering. *Scientific Reports*, **2013**, 3, 2011	4.9	3
14	Electron–phonon coupling and charge-transfer excitations in organic systems from many-body perturbation theory. *Journal of Materials Science*, **2012**, 47, 7472-7481	4.3	27
13	Short-range to long-range charge-transfer excitations in the zincbacteriochlorin-bacteriochlorin complex: a Bethe-Salpeter study. *Physical Review Letters*, **2012**, 109, 167801	7.4	85
12	Many-body Green function study of coumarins for dye-sensitized solar cells. *Physical Review B*, **2012**, 86,	3.3	48
11	Atomistic simulations of heat transport in real-scale silicon nanowire devices. *Applied Physics Letters*, **2012**, 100, 223107	3.4	11
10	Atomistic calculation of the thermal conductance of large scale bulk-nanowire junctions. *Physical Review B*, **2011**, 84,	3.3	17
9	Single OR molecule and OR atomic circuit logic gates interconnected on a Si(100)H surface. *Journal of Physics Condensed Matter*, **2011**, 23, 125303	1.8	26
8	Ab initio investigation of the melting line of nitrogen at high pressure. *Physical Review B*, **2010**, 82,	3.3	25
7	A scalable and accurate algorithm for the computation of Hartree–Fock exchange. *Computer Physics Communications*, **2010**, 181, 855-860	4.2	38
6	Practical algorithms to facilitate large-scale first-principles molecular dynamics. *Journal of Physics: Conference Series*, **2009**, 180, 012074	0.3	6
5	Calculation of the conductance of a finite atomic line of sulfur vacancies created on a molybdenum disulfide surface. *Physical Review B*, **2008**, 77,	3.3	39
4	An intramolecular digital 1/2-adder with tunneling current drive and read-outs. *Chemical Physics Letters*, **2008**, 452, 269-274	2.5	24
3	A quantum digital half adder inside a single molecule. *Chemical Physics Letters*, **2005**, 406, 167-172	2.5	41
2	HAMILTONIAN LOGIC GATES: COMPUTING INSIDE A MOLECULE. *International Journal of Nanoscience*, **2005**, 04, 107-118	0.6	4

1 Intramolecular Hamiltonian logic gates. *Physica E: Low-Dimensional Systems and Nanostructures*, **2004**, 24, 161-172 3 20