

Ivan Duchemin

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72
papers

2,387
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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	0-0 Energies Using Hybrid Schemes: Benchmarks of TD-DFT, CIS(D), ADC(2), CC2, and BSE/GW formalisms for 80 Real-Life Compounds. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5340-59	6.4	166
71	Benchmarking the Bethe-Salpeter Formalism on a Standard Organic Molecular Set. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 3290-304	6.4	145
70	The Bethe-Salpeter equation in chemistry: relations with TD-DFT, applications and challenges. <i>Chemical Society Reviews</i> , 2018 , 47, 1022-1043	58.5	110
69	Benchmark Many-Body GW and Bethe-Salpeter Calculations for Small Transition Metal Molecules. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3934-43	6.4	87
68	Short-range to long-range charge-transfer excitations in the zincbacteriochlorin-bacteriochlorin complex: a Bethe-Salpeter study. <i>Physical Review Letters</i> , 2012 , 109, 167801	7.4	85
67	Excited states properties of organic molecules: from density functional theory to the GW and Bethe-Salpeter Green@ function formalisms. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2014 , 372, 20130271	3	81
66	Fast and Accurate Electronic Excitations in Cyanines with the Many-Body Bethe-Salpeter Approach. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 1212-8	6.4	73
65	1.9% bi-axial tensile strain in thick germanium suspended membranes fabricated in optical germanium-on-insulator substrates for laser applications. <i>Applied Physics Letters</i> , 2015 , 107, 191904	3.4	62
64	Is the Bethe-Salpeter Formalism Accurate for Excitation Energies? Comparisons with TD-DFT, CASPT2, and EOM-CCSD. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 1524-1529	6.4	61
63	Combining the Many-Body GW Formalism with Classical Polarizable Models: Insights on the Electronic Structure of Molecular Solids. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 2814-20	6.4	59
62	Few-electron edge-state quantum dots in a silicon nanowire field-effect transistor. <i>Nano Letters</i> , 2014 , 14, 2094-8	11.5	54
61	Benchmark of Bethe-Salpeter for Triplet Excited-States. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 767-783	6.4	51
60	First Principles Calculations of Charge Transfer Excitations in PolymerBullerene Complexes: Influence of Excess Energy. <i>Advanced Functional Materials</i> , 2015 , 25, 1972-1984	15.6	50
59	Many-body Green@ function study of coumarins for dye-sensitized solar cells. <i>Physical Review B</i> , 2012 , 86,	3.3	48
58	Mechanical Tuning of Thermal Transport in a Molecular Junction. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 24636-24642	3.8	44
57	Host dependence of the electron affinity of molecular dopants. <i>Materials Horizons</i> , 2019 , 6, 107-114	14.4	44
56	Many-body Green@ function GW and Bethe-Salpeter study of the optical excitations in a paradigmatic model dipeptide. <i>Journal of Chemical Physics</i> , 2013 , 139, 194308	3.9	44

55	Resonant hot charge-transfer excitations in fullerene-porphyrin complexes: Many-body Bethe-Salpeter study. <i>Physical Review B</i> , 2013 , 87,	3.3	43
54	Efficient Computation of Hartree-Fock Exchange Using Recursive Subspace Bisection. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 582-7	6.4	42
53	A quantum digital half adder inside a single molecule. <i>Chemical Physics Letters</i> , 2005 , 406, 167-172	2.5	41
52	Calculation of the conductance of a finite atomic line of sulfur vacancies created on a molybdenum disulfide surface. <i>Physical Review B</i> , 2008 , 77,	3.3	39
51	Germanium under High Tensile Stress: Nonlinear Dependence of Direct Band Gap vs Strain. <i>ACS Photonics</i> , 2016 , 3, 1907-1911	6.3	39
50	A Strategy to Suppress Phonon Transport in Molecular Junctions Using π -Stacked Systems. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 7175-7182	3.8	38
49	Quantum calculations of the carrier mobility: Methodology, Matthiessen's rule, and comparison with semi-classical approaches. <i>Journal of Applied Physics</i> , 2014 , 115, 054512	2.5	38
48	A scalable and accurate algorithm for the computation of Hartree-Fock exchange. <i>Computer Physics Communications</i> , 2010 , 181, 855-860	4.2	38
47	The Bethe-Salpeter Equation Formalism: From Physics to Chemistry. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 7371-7382	6.4	38
46	The Bethe-Salpeter formalism with polarisable continuum embedding: reconciling linear-response and state-specific features. <i>Chemical Science</i> , 2018 , 9, 4430-4443	9.4	37
45	Accurate description of charged excitations in molecular solids from embedded many-body perturbation theory. <i>Physical Review B</i> , 2018 , 97,	3.3	34
44	Assessment of the Accuracy of the Bethe-Salpeter (BSE/GW) Oscillator Strengths. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 3969-81	6.4	34
43	Correlated electron-hole mechanism for molecular doping in organic semiconductors. <i>Physical Review Materials</i> , 2017 , 1,	3.2	31
42	GW and Bethe-Salpeter study of small water clusters. <i>Journal of Chemical Physics</i> , 2016 , 144, 034109	3.9	31
41	Combining the Bethe-Salpeter Formalism with Time-Dependent DFT Excited-State Forces to Describe Optical Signatures: NBO Fluoroborates as Working Examples. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 4548-56	6.4	30
40	Does Excess Energy Assist Photogeneration in an Organic Low-Bandgap Solar Cell?. <i>Advanced Functional Materials</i> , 2015 , 25, 1287-1295	15.6	30
39	Combining the GW formalism with the polarizable continuum model: A state-specific non-equilibrium approach. <i>Journal of Chemical Physics</i> , 2016 , 144, 164106	3.9	30
38	Electron-phonon coupling and charge-transfer excitations in organic systems from many-body perturbation theory. <i>Journal of Materials Science</i> , 2012 , 47, 7472-7481	4.3	27

37	Single OR molecule and OR atomic circuit logic gates interconnected on a Si(100)H surface. <i>Journal of Physics Condensed Matter</i> , 2011 , 23, 125303	1.8	26
36	Accurate strain measurements in highly strained Ge microbridges. <i>Applied Physics Letters</i> , 2016 , 108, 241902	3.4	26
35	Exploring approximations to the GW self-energy ionic gradients. <i>Physical Review B</i> , 2015 , 91,	3.3	25
34	Ab initio investigation of the melting line of nitrogen at high pressure. <i>Physical Review B</i> , 2010 , 82,	3.3	25
33	Quantum dot made in metal oxide silicon-nanowire field effect transistor working at room temperature. <i>Nano Letters</i> , 2015 , 15, 2958-64	11.5	24
32	An intramolecular digital 1/2-adder with tunneling current drive and read-outs. <i>Chemical Physics Letters</i> , 2008 , 452, 269-274	2.5	24
31	Robust Analytic-Continuation Approach to Many-Body Calculations. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 1742-1756	6.4	23
30	Separable resolution-of-the-identity with all-electron Gaussian bases: Application to cubic-scaling RPA. <i>Journal of Chemical Physics</i> , 2019 , 150, 174120	3.9	23
29	Quantum Modeling of the Carrier Mobility in FDSOI Devices. <i>IEEE Transactions on Electron Devices</i> , 2014 , 61, 3096-3102	2.9	20
28	Intramolecular Hamiltonian logic gates. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2004 , 24, 161-172	3	20
27	Bethe-Salpeter study of cationic dyes: Comparisons with ADC(2) and TD-DFT. <i>Journal of Chemical Physics</i> , 2017 , 146, 034301	3.9	18
26	Calculations of n- π Transition Energies: Comparisons Between TD-DFT, ADC, CC, CASPT2, and BSE/GW Descriptions. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 6122-6134	2.8	17
25	Atomistic calculation of the thermal conductance of large scale bulk-nanowire junctions. <i>Physical Review B</i> , 2011 , 84,	3.3	17
24	Cubic-Scaling All-Electron Calculations with a Separable Density-Fitting Space-Time Approach. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 2383-2393	6.4	17
23	Assessment of the convergence of partially self-consistent BSE/GW calculations. <i>Molecular Physics</i> , 2016 , 114, 957-967	1.7	16
22	Helium Atom Excitations by the GW and Bethe-Salpeter Many-Body Formalism. <i>Physical Review Letters</i> , 2017 , 118, 163001	7.4	16
21	Hybrid and Constrained Resolution-of-Identity Techniques for Coulomb Integrals. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 1199-1208	6.4	15
20	Pros and Cons of the Bethe-Salpeter Formalism for Ground-State Energies. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 3536-3545	6.4	15

19	Modeling the Photochrome-TiO Interface with Bethe-Salpeter and Time-Dependent Density Functional Theory Methods. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 936-940	6.4	14
18	Study of the light emission in Ge layers and strained membranes on Si substrates. <i>Thin Solid Films</i> , 2016 , 613, 64-67	2.2	14
17	Magnetotransport subband spectroscopy in InAs nanowires. <i>Physical Review Letters</i> , 2014 , 112, 076801	7.4	14
16	Phonon-limited carrier mobility and resistivity from carbon nanotubes to graphene. <i>Physical Review B</i> , 2015 , 92,	3.3	11
15	Atomistic simulations of heat transport in real-scale silicon nanowire devices. <i>Applied Physics Letters</i> , 2012 , 100, 223107	3.4	11
14	Ground-state correlation energy of beryllium dimer by the Bethe-Salpeter equation. <i>SciPost Physics</i> , 2020 , 8,	6.1	8
13	Multi-scale strategy for high-k/metal-gate UTBB-FDSOI devices modeling with emphasis on back bias impact on mobility. <i>Journal of Computational Electronics</i> , 2013 , 12, 675-684	1.8	6
12	Practical algorithms to facilitate large-scale first-principles molecular dynamics. <i>Journal of Physics: Conference Series</i> , 2009 , 180, 012074	0.3	6
11	Accurate complex scaling of three dimensional numerical potentials. <i>Journal of Chemical Physics</i> , 2013 , 138, 204111	3.9	5
10	Study of the piezoresistive properties of NMOS and PMOS Egate SOI nanowire transistors: Scalability effects and high stress level 2014 ,		5
9	HAMILTONIAN LOGIC GATES: COMPUTING INSIDE A MOLECULE. <i>International Journal of Nanoscience</i> , 2005 , 04, 107-118	0.6	4
8	Remote surface roughness scattering in fully depleted silicon-on-insulator devices with high- γ SiO ₂ gate stacks. <i>Applied Physics Letters</i> , 2015 , 106, 023508	3.4	3
7	Mobility in high-K metal gate UTBB-FDSOI devices: From NEGF to TCAD perspectives 2013 ,		3
6	Metallic behaviour in SOI quantum wells with strong intervalley scattering. <i>Scientific Reports</i> , 2013 , 3, 2011	4.9	3
5	Optical properties of graphene quantum dots: the role of chiral symmetry. <i>2D Materials</i> , 2020 , 7, 0250415.9	15.9	2
4	Revealing the band structure of InSb nanowires by high-field magnetotransport in the quasiballistic regime. <i>Physical Review B</i> , 2016 , 94,	3.3	2
3	Photoluminescent properties of the carbon-dimer defect in hexagonal boron-nitride: A many-body finite-size cluster approach. <i>Physical Review Materials</i> , 2021 , 5,	3.2	2
2	Non-linear model of electronic band structure to highly tensile-strained Germanium 2015 ,		1

1 Modeling of the Bandgap Distribution in Bi-Axially Strained Germanium Crossbeam for Laser Applications. *IEEE Photonics Journal*, **2022**, 14, 1-4

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