Gustavo E Scuseria

List of Publications by Citations

274 papers	51,882 citations	83 h-index	226 g-index
400 ext. papers	57,321 ext. citations	5.4 avg, IF	7.93 L-index

#	Paper	IF	Citations
274	Hybrid functionals based on a screened Coulomb potential. *Journal of Chemical Physics*, **2003**, 118, 8207-8215	3.9	10573
273	Climbing the density functional ladder: nonempirical meta-generalized gradient approximation designed for molecules and solids. *Physical Review Letters*, **2003**, 91, 146401	7.4	4737
272	Assessment of the PerdewBurkeErnzerhof exchange-correlation functional. *Journal of Chemical Physics*, **1999**, 110, 5029-5036	3.9	2906
271	Comparative assessment of a new nonempirical density functional: Molecules and hydrogen-bonded complexes. *Journal of Chemical Physics*, **2003**, 119, 12129-12137	3.9	1724
270	Efficient hybrid density functional calculations in solids: assessment of the Heyd-Scuseria-Ernzerhof screened Coulomb hybrid functional. *Journal of Chemical Physics*, **2004**, 121, 1187-92	3.9	1520
269	An efficient reformulation of the closed-shell coupled cluster single and double excitation (CCSD) equations. *Journal of Chemical Physics*, **1988**, 89, 7382-7387	3.9	1382
268	Assessment of a long-range corrected hybrid functional. *Journal of Chemical Physics*, **2006**, 125, 234109	3.9	1356
267	Energy band gaps and lattice parameters evaluated with the Heyd-Scuseria-Ernzerhof screened hybrid functional. *Journal of Chemical Physics*, **2005**, 123, 174101	3.9	1306
266	Is coupled cluster singles and doubles (CCSD) more computationally intensive than quadratic configuration interaction (QCISD)?. *Journal of Chemical Physics*, **1989**, 90, 3700-3703	3.9	956
265	Importance of short-range versus long-range Hartree-Fock exchange for the performance of hybrid density functionals. *Journal of Chemical Physics*, **2006**, 125, 074106	3.9	747
264	TD-DFT Performance for the Visible Absorption Spectra of Organic Dyes: Conventional versus Long-Range Hybrids. *Journal of Chemical Theory and Computation*, **2008**, 4, 123-35	6.4	681
263	A novel form for the exchange-correlation energy functional. *Journal of Chemical Physics*, **1998**, 109, 400-410	3.9	661
262	Prescription for the design and selection of density functional approximations: more constraint satisfaction with fewer fits. *Journal of Chemical Physics*, **2005**, 123, 62201	3.9	658
261	Assessment and validation of a screened Coulomb hybrid density functional. *Journal of Chemical Physics*, **2004**, 120, 7274-80	3.9	569
260	Tests of functionals for systems with fractional electron number. *Journal of Chemical Physics*, **2007**, 126, 154109	3.9	503
259	The indirect to direct band gap transition in multilayered MoS2 as predicted by screened hybrid density functional theory. *Applied Physics Letters*, **2011**, 99, 261908	3.4	431
258	Linear Scaling Density Functional Calculations with Gaussian Orbitals. *Journal of Physical Chemistry A*, **1999**, 103, 4782-4790	2.8	372

257	Analytic evaluation of energy gradients for the single and double excitation coupled cluster (CCSD) wave function: Theory and application. *Journal of Chemical Physics*, **1987**, 87, 5361-5373	3.9	358
256	Meta-generalized gradient approximation: explanation of a realistic nonempirical density functional. *Journal of Chemical Physics*, **2004**, 120, 6898-911	3.9	355
255	Spurious fractional charge on dissociated atoms: pervasive and resilient self-interaction error of common density functionals. *Journal of Chemical Physics*, **2006**, 125, 194112	3.9	349
254	Linear scaling second-order MollerPlesset theory in the atomic orbital basis for large molecular systems. *Journal of Chemical Physics*, **1999**, 110, 3660-3671	3.9	349
253	Screened hybrid density functionals for solid-state chemistry and physics. *Physical Chemistry Chemical Physics*, **2009**, 11, 443-54	3.6	331
252	Can short-range hybrids describe long-range-dependent properties?. *Journal of Chemical Physics*, **2009**, 131, 044108	3.9	322
251	The closed-shell coupled cluster single and double excitation (CCSD) model for the description of electron correlation. A comparison with configuration interaction (CISD) results. *Journal of Chemical Physics*, **1987**, 86, 2881-2890	3.9	291
250	Linear scaling coupled cluster and perturbation theories in the atomic orbital basis. *Journal of Chemical Physics*, **1999**, 111, 8330-8343	3.9	290
249	Predicting Band Gaps with Hybrid Density Functionals. *Journal of Physical Chemistry Letters*, **2016**, 7, 4165-4170	6.4	286
248	Understanding band gaps of solids in generalized Kohn-Sham theory. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 2801-2806	11.5	280
247	Half-metallic graphene nanodots: A comprehensive first-principles theoretical study. *Physical Review B*, **2008**, 77,	3.3	271
246	Solutions of the Two-Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms. *Physical Review X*, **2015**, 5,	9.1	269
245	Local hybrid functionals. *Journal of Chemical Physics*, **2003**, 118, 1068-1073	3.9	255
244	Covalency in the actinide dioxides: Systematic study of the electronic properties using screened hybrid density functional theory. *Physical Review B*, **2007**, 76,	3.3	248
243	Density functionals that are one- and two- are not always many-electron self-interaction-free, as shown for H2+, He2+, LiH+, and Ne2+. *Journal of Chemical Physics*, **2007**, 126, 104102	3.9	248
242	The ground state correlation energy of the random phase approximation from a ring coupled cluster doubles approach. *Journal of Chemical Physics*, **2008**, 129, 231101	3.9	239
241	Analytic evaluation of energy gradients for the singles and doubles coupled cluster method including perturbative triple excitations: Theory and applications to FOOF and Cr2. *Journal of Chemical Physics*, **1991**, 94, 442-447	3.9	238
240	Linear scaling conjugate gradient density matrix search as an alternative to diagonalization for first principles electronic structure calculations. *Journal of Chemical Physics*, **1997**, 106, 5569-5577	3.9	229

239	Accurate treatment of solids with the HSE screened hybrid. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 767-774	1.3	216
238	Coupled cluster energy derivatives. Analytic Hessian for the closed-shell coupled cluster singles and doubles wave function: Theory and applications. *Journal of Chemical Physics*, **1990**, 92, 4924-4940	3.9	214
237	Generalized gradient approximation model exchange holes for range-separated hybrids. *Journal of Chemical Physics*, **2008**, 128, 194105	3.9	200
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235	Role of sp3 carbon and 7-membered rings in fullerene annealing and fragmentation. *Nature*, **1993**, 366, 665-667	50.4	181
234	Atomic orbital Laplace-transformed second-order M□ller□Plesset theory for periodic systems. *Journal of Chemical Physics*, **2001**, 115, 9698-9707	3.9	180
233	Projected Hartree-Fock theory. *Journal of Chemical Physics*, **2012**, 136, 164109	3.9	174
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231	Comparison of coupled-cluster results with a hybrid of Hartree□Fock and density functional theory. *Journal of Chemical Physics*, **1992**, 97, 7528-7530	3.9	164
230	Long-range-corrected hybrids including random phase approximation correlation. *Journal of Chemical Physics*, **2009**, 130, 081105	3.9	152
229	Ab initio theoretical predictions of C28, C28H4, C28F4, (Ti@C28)H4, and M@C28 (M=Mg, Al, Si, S, Ca, Sc, Ti, Ge, Zr, and Sn). *Journal of Chemical Physics*, **1993**, 99, 352-359	3.9	149
228	The vibrational frequencies of ozone. *Journal of Chemical Physics*, **1990**, 93, 489-494	3.9	149
227	Density functionals that recognize covalent, metallic, and weak bonds. *Physical Review Letters*, **2013**, 111, 106401	7.4	143
226	Edge effects in finite elongated graphene nanoribbons. *Physical Review B*, **2007**, 76,	3.3	143
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224	The importance of middle-range Hartree-Fock-type exchange for hybrid density functionals. *Journal of Chemical Physics*, **2007**, 127, 221103	3.9	139
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220	Projected quasiparticle theory for molecular electronic structure. *Journal of Chemical Physics*, **2011**, 135, 124108	3.9	130
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217	Mechanically induced defects and strength of BN nanotubes. *Physical Review B*, **2002**, 65,	3.3	124
216	A quantitative study of the scaling properties of the Hartree-Fock method. *Journal of Chemical Physics*, **1995**, 102, 8448-8452	3.9	123
215	Towards the Solution of the Many-Electron Problem in Real Materials: Equation of State of the Hydrogen Chain with State-of-the-Art Many-Body Methods. *Physical Review X*, **2017**, 7,	9.1	121
214	Seniority zero pair coupled cluster doubles theory. *Journal of Chemical Physics*, **2014**, 140, 214113	3.9	119
213	Comparison of screened hybrid density functional theory to diffusion Monte Carlo in calculations of total energies of silicon phases and defects. *Physical Review B*, **2006**, 74,	3.3	119
212	Hybrid functionals including random phase approximation correlation and second-order screened exchange. *Journal of Chemical Physics*, **2010**, 132, 094103	3.9	117
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202	Doping of polyaniline by acid-base chemistry: density functional calculations with periodic boundary conditions. *Journal of the American Chemical Society*, **2005**, 127, 11318-27	16.4	95
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197	Density matrix embedding from broken symmetry lattice mean fields. *Physical Review B*, **2014**, 89,	3.3	90
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176	Exact parameterization of fermionic wave functions via unitary coupled cluster theory. *Journal of Chemical Physics*, **2019**, 151, 244112	3.9	63
175	Thermodynamics of yield in boron nitride nanotubes. *Physical Review B*, **2003**, 68,	3.3	62
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106	The role of the reference state in long-range random phase approximation correlation. *Journal of Chemical Physics*, **2009**, 131, 154106	3.9	28
105	Coulomb-only second-order perturbation theory in long-range-corrected hybrid density functionals. *Physical Chemistry Chemical Physics*, **2009**, 11, 9677-86	3.6	28
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