Kevin E Riley

List of Publications by Year
in descending order

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43 papers	5,408 citations	236612 25 h-index	276539 41 g-index
43 all docs	43 docs citations	43 times ranked	4530 citing authors

#	Article	IF	Citations
1	Fentanyl Assay Derived from Intermolecular Interaction-Enabled Small Molecule Recognition (iMSR) with Differential Impedance Analysis for Point-of-Care Testing. Analytical Chemistry, 2022, 94, 9242-9251.	3.2	7
2	The quantum pencil revisited. European Journal of Physics, 2021, 42, 065406.	0.3	0
3	Critical comparison of R Xâ‹¯Y and R Hâ‹¯Y directionality in halogen and hydrogen bonds using modern computational chemistry methods. Chemical Physics Letters, 2020, 744, 137221.	1.2	10
4	Câ€“D Vibration at C2 Position of Imidazolium Cation as a Probe of the Ionic Liquid Microenvironment. Journal of Physical Chemistry A, 2019, 123, 6342-6349.	1.1	10
5	Point-of-Care Determination of Acetaminophen Levels with Multi-Hydrogen Bond Manipulated Single-Molecule Recognition (eMuHSiR). Analytical Chemistry, 2018, 90, 4733-4740.	3.2	25
6	Crystal structures of the hexafluoridophosphate salts of the isomeric 2-, 3- and 4-cyano-1-methylpyridinium cations and determination of solid-state interaction energies. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1322-1329.	0.2	0
7	Osteoinductive effects of glyceollins on adult mesenchymal stromal/stem cells from adipose tissue and bone marrow. Phytomedicine, 2017, 27, 39-51.	2.3	15
8	Strength, character, and directionality of halogen bonds involving cationic halogen bond donors. Faraday Discussions, 2017, 203, 47-60.	1.6	21
9	Ligands of Therapeutic Utility for the Liver X Receptors. Molecules, 2017, 22, 88.	1.7	67
10	Strength and Character of Râ€“XÂ·Â·Â·Ï€ Interactions Involving Aromatic Amino Acid Sidechains in Protein-Ligand Complexes Derived from Crystal Structures in the Protein Data Bank. Crystals, 2017, 7, 273.	1.0	15
11	Exploring the (Very Flat) Potential Energy Landscape of Râˆ™Brâ‹…â‹…â‹…â‹…Ï€ Interactions with Accurate CCSD(T) and SAPT Techniques. Chemistry - A European Journal, 2016, 22, 17690-17695.	1.7	21
12	Comparative analysis of electrostatic potential maxima and minima on molecular surfaces, as determined by three methods and a variety of basis sets. Journal of Computational Science, 2016, 17, 273-284.	1.5	62
13	Comparison of hydrogen bonds, halogen bonds, C Hâ‹¯Ï€ interactions, and C Xâ‹¯Ï€ interactions using high-level ab initio methods. Chemical Physics Letters, 2015, 621, 165-170.	1.2	49
14	On the Importance and Origin of Aromatic Interactions in Chemistry and Biodisciplines. Accounts of Chemical Research, 2013, 46, 927-936.	7.6	206
15	The relative roles of electrostatics and dispersion in the stabilization of halogen bonds. Physical Chemistry Chemical Physics, 2013, 15, 17742.	1.3	129
16	Competition between halogen, dihalogen and hydrogen bonds in bromo- and iodomethanol dimers. Journal of Molecular Modeling, 2013, 19, 2879-2883.	0.8	18
17	Basis Set Dependence of Interaction Energies Computed Using Composite Post-MP2 Methods. Journal of Chemical Theory and Computation, 2013, 9, 330-337.	2.3	12
18	Halogen bond tunability II: the varying roles of electrostatic and dispersion contributions to attraction in halogen bonds. Journal of Molecular Modeling, 2013, 19, 4651-4659.	0.8	190

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19	Assessment of the Performance of MP2 and MP2 Variants for the Treatment of Noncovalent Interactions. Journal of Physical Chemistry A, 2012, 116, 4159-4169.	1.1	107
20	The performance of MP2.5 and MP2.X methods for nonequilibrium geometries of molecular complexes. Physical Chemistry Chemical Physics, 2012, 14, 13187.	1.3	20
21	Benchmark Calculations of Noncovalent Interactions of Halogenated Molecules. Journal of Chemical Theory and Computation, 2012, 8, 4285-4292.	2.3	264
22	Polarization-induced Ïƒ-holes and hydrogen bonding. Journal of Molecular Modeling, 2012, 18, 2461-2469.	0.8	121
23	MP2.X: a generalized MP2.5 method that produces improved binding energies with smaller basis sets. Physical Chemistry Chemical Physics, 2011, 13, 21121.	1.3	41
24	S66: A Well-balanced Database of Benchmark Interaction Energies Relevant to Biomolecular Structures. Journal of Chemical Theory and Computation, 2011, 7, 2427-2438.	2.3	821
25	Complete Basis Set Extrapolation and Hybrid Schemes for Geometry Gradients of Noncovalent Complexes. Journal of Chemical Theory and Computation, 2011, 7, 3924-3934.	2.3	24
26	Extensions of the S66 Data Set: More Accurate Interaction Energies and Angular-Displaced Nonequilibrium Geometries. Journal of Chemical Theory and Computation, 2011, 7, 3466-3470.	2.3	201
27	Strength and Character of Halogen Bonds in Proteinâ€“Ligand Complexes. Crystal Growth and Design, 2011, 11, 4272-4278.	1.4	84
28	Dispersion-corrected density functional theory comparison of hydrogen adsorption on boron-nitride and carbon nanotubes. Physical Review B, 2011, 84, .	1.1	24
29	Noncovalent interactions in biochemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 3-17.	6.2	222
30	Halogen bond tunability I: the effects of aromatic fluorine substitution on the strengths of halogen-bonding interactions involving chlorine, bromine, and iodine. Journal of Molecular Modeling, 2011, 17, 3309-3318.	0.8	374
31	What is the best density functional to describe water clusters: evaluation of widely used density functionals with various basis sets for (H2O) n (nÂ=Â1â€“10). Theoretical Chemistry Accounts, 2011, 130, 341-352.	0.5	46
32	Ab initio studies of the characteristics of hydrogen bonds involving aromatically bound hydroxyl and amino groups and the effects of aromatic fluorine substitution on these interactions. International Journal of Quantum Chemistry, 2010, 110, 1833-1841.	1.0	4
33	On the Structure and Geometry of Biomolecular Binding Motifs (Hydrogen-Bonding, Stacking, Xâ‹¯HÂ·Â·Â·Ï€): WFT and DFT Calculations. Journal of Chemical Theory and Computation, 2010, 6, 66-80.	2.3	175
34	Stabilization and Structure Calculations for Noncovalent Interactions in Extended Molecular Systems Based on Wave Function and Density Functional Theories. Chemical Reviews, 2010, 110, 5023-5063.	23.0	697
35	Directional Weak Intermolecular Interactions: Ïƒ-Hole Bonding. Australian Journal of Chemistry, 2010, 63, 1598.	0.5	235
36	Reference Quantum Chemical Calculations on RNA Base Pairs Directly Involving the 2â€²-OH Group of Ribose. Journal of Chemical Theory and Computation, 2009, 5, 1166-1179.	2.3	27

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37	Representative Amino Acid Side Chain Interactions in Proteins. A Comparison of Highly Accurate Correlatedab InitioQuantum Chemical and Empirical Potential Procedures. Journal of Chemical Theory and Computation, 2009, 5, 982-992.	2.3	89
38	BrÂ·Â·Â·O Complexes as Probes of Factors Affecting Halogen Bonding: Interactions of Bromobenzenes and Bromopyrimidines with Acetone. Journal of Chemical Theory and Computation, 2009, 5, 155-163.	2.3	303
39	Investigations into the Nature of Halogen Bonding Including Symmetry Adapted Perturbation Theory Analyses. Journal of Chemical Theory and Computation, 2008, 4, 232-242.	2.3	403
40	A DFTâ˜'D Investigation of the Mechanisms for Activation of the Wild-Type and S810L Mutated Mineralocorticoid Receptor by Steroid Hormones. Journal of Physical Chemistry B, 2008, 112, 3157-3163.	1.2	14
41	Assessment of the MP2 Method, along with Several Basis Sets, for the Computation of Interaction Energies of Biologically Relevant Hydrogen Bonded and Dispersion Bound Complexes. Journal of Physical Chemistry A, 2007, 111, 8257-8263.	1.1	170
42	Performance of the DFT-D method, paired with the PCM implicit solvation model, for the computation of interaction energies of solvated complexes of biological interest. Physical Chemistry Chemical Physics, 2007, 9, 5555.	1.3	63
43	Role of Solvation in the Energy Stabilization Inside the Hydrophobic Core of the Protein Rubredoxin. Journal of Physical Chemistry B, 2006, 110, 15650-15653.	1.2	22