# Joanna Sadlej

## List of Publications by Year in descending order

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|---|---|---|---|
| 114 papers | 5,669 citations | 147801 31 h-index | 76900 74 g-index |
| 123 all docs | 123 docs citations | 123 times ranked | 5388 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | An excursion into secondary pharmacology of fentanyls with potential implications for drug design: Ïƒ1 receptor. , 2022, , 89-100. | | 0 |
| 2 | Towards Quantum-Chemical Modeling of the Activity of Anesthetic Compounds. International Journal of Molecular Sciences, 2021, 22, 9272. | 4.1 | 3 |
| 3 | Affinity of fentanyl and its derivatives for the Ïƒ1-receptor. MedChemComm, 2019, 10, 1187-1191. | 3.4 | 10 |
| 4 | Fentanyl Family at the Mu-Opioid Receptor: Uniform Assessment of Binding and Computational Analysis. Molecules, 2019, 24, 740. | 3.8 | 39 |
| 5 | The influence of the dispersion corrections on the performance of DFT method in modeling HNgY noble gas molecules and their complexes. Chemical Physics Letters, 2018, 691, 319-324. | 2.6 | 7 |
| 6 | Molecular dynamics simulations suggest why the A2058G mutation in 23S RNA results in bacterial resistance against clindamycin. Journal of Molecular Modeling, 2018, 24, 191. | 1.8 | 7 |
| 7 | Structural Insights into Ïƒ1 Receptor Interactions with Opioid Ligands by Molecular Dynamics Simulations. Molecules, 2018, 23, 456. | 3.8 | 3 |
| 8 | Tailoring the Schiff base photoswitching â€“ a non-adiabatic molecular dynamics study of substituent effect on excited state proton transfer. Physical Chemistry Chemical Physics, 2017, 19, 5318-5325. | 2.8 | 30 |
| 9 | The FMO analysis of the molecular interaction of fentanyl derivatives with the Î¼-opioid receptor. Chemical Papers, 2017, 71, 1429-1443. | 2.2 | 7 |
| 10 | Conformational space of clindamycin studied by ab initio and full-atom molecular dynamics. Journal of Molecular Modeling, 2016, 22, 20. | 1.8 | 2 |
| 11 | Î±-Amino Acids In Water: A Review Of VCD And ROA Spectra. Challenges and Advances in Computational Chemistry and Physics, 2014, , 83-160. | 0.6 | 2 |
| 12 | Calculations of NMR properties for sI and sII clathrate hydrates of carbon dioxide. Chemical Physics, 2014, 433, 31-41. | 1.9 | 10 |
| 13 | Calculations of NMR properties for sI and sII clathrate hydrates of methane, ethane and propane. Journal of Molecular Modeling, 2014, 20, 2511. | 1.8 | 7 |
| 14 | Excitedâ€State Intramolecular Proton Transfer: Photoswitching in Salicylidene Methylamine Derivatives. ChemPhysChem, 2014, 15, 1643-1652. | 2.1 | 49 |
| 15 | Prediction ofl-Methionine VCD Spectra in the Gas Phase and Water Solution. Journal of Physical Chemistry B, 2013, 117, 14202-14214. | 2.6 | 19 |
| 16 | Recent Advances in Spectroscopy of Hydrogen-Bonded Systems. Journal of Atomic, Molecular, and Optical Physics, 2012, 2012, 1-1. | 0.5 | 1 |
| 17 | Photophysics of Schiff Bases: Theoretical Study of Salicylidene Methylamine. ChemPhysChem, 2012, 13, 4287-4294. | 2.1 | 45 |
| 18 | On Vibrational Circular Dichroism Chirality Transfer in Electron Donorâ€“Acceptor Complexes: A Prediction for the QuinineÂ·Â·Â·BF‹sub›3‹/sub› System. Journal of Physical Chemistry A, 2012, 116, 7916-7926. | 2.5 | 13 |

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|---|---|---|---|
| 19 | Computational study on interaction energy changes during double proton transfer process. Computational and Theoretical Chemistry, 2012, 998, 120-128. | 2.5 | 4 |
| 20 | Thermal Fluctuations and Infrared Spectra of the Formamideâ€“Formamidine Complex. Journal of Physical Chemistry A, 2012, 116, 10412-10419. | 2.5 | 4 |
| 21 | Inverse hydrogen bond: theoretical investigation on the nature of interaction and spectroscopic properties. Structural Chemistry, 2012, 23, 1323-1332. | 2.0 | 10 |
| 22 | Quantum mechanical studies of lincosamides. Journal of Molecular Modeling, 2012, 18, 2727-2740. | 1.8 | 6 |
| 23 | Calculated Nuclear Magnetic Resonance Parameters for Multiproton-Exchange and Nonbonded-Hydrogen Rotation Processes in Cyclic Water Clusters. Journal of Physical Chemistry A, 2011, 115, 5774-5784. | 2.5 | 2 |
| 24 | Nuclear Magnetic Resonance Parameters for Methane Molecule Trapped in Clathrate Hydrates. Journal of Physical Chemistry A, 2011, 115, 612-619. | 2.5 | 20 |
| 25 | Theoretical predictions of the spectroscopic parameters in noble-gas molecules: HXeOH and its complex with water. Physical Chemistry Chemical Physics, 2011, 13, 15455. | 2.8 | 13 |
| 26 | VCD Chirality Transfer: A New Insight into the Intermolecular Interactions. , 2011, , 451-478. | | 4 |
| 27 | Definition of the hydrogen bond (IUPAC Recommendations 2011). Pure and Applied Chemistry, 2011, 83, 1637-1641. | 1.9 | 1,449 |
| 28 | Defining the hydrogen bond: An account (IUPAC Technical Report). Pure and Applied Chemistry, 2011, 83, 1619-1636. | 1.9 | 856 |
| 29 | Spectroscopic parameters in noble gas molecule: HXeF and its complex with HF. Chemical Physics Letters, 2011, 517, 155-161. | 2.6 | 11 |
| 30 | Phenylisoserine in the gas-phase and water: Ab initio studies on neutral and zwitterion conformers. Journal of Molecular Modeling, 2011, 17, 961-970. | 1.8 | 9 |
| 31 | Ab initio simulations of the NMR spectra of Î²-alanine conformers. Computational and Theoretical Chemistry, 2011, 964, 148-154. | 2.5 | 9 |
| 32 | VCD spectroscopy as a novel probe for chirality transfer in molecular interactions. Chemical Society Reviews, 2010, 39, 1478-1488. | 38.1 | 118 |
| 33 | Theoretical Study of the Lactic Acidâ^'Water System: Importance of Two- and Three-Body Interactions. Journal of Physical Chemistry A, 2010, 114, 4427-4436. | 2.5 | 4 |
| 34 | IR low-temperature matrix, X-ray and ab initio study on l-isoserine conformations. Physical Chemistry Chemical Physics, 2010, 12, 10818. | 2.8 | 22 |
| 35 | The water-nitric oxide intermolecular potential-energy surface revisited. Journal of Chemical Physics, 2009, 130, 104303. | 3.0 | 22 |
| 36 | Static electric polarizabilities and first hyperpolarizabilities of molecular ions RgH+ (Rg=He, Ne, Ar,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 | 2.6 | 6 |

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|---|---|---|---|
| 37 | A computational study of the nuclear magnetic resonance parameters for double proton exchange pathways in the formamideâ€“formic acid and formamideâ€“formamidine complexes. Physical Chemistry Chemical Physics, 2009, 11, 11232. | 2.8 | 12 |
| 38 | IR Lowâ€Temperature Matrix and ab Initio Study on Î²â€Alanine Conformers. ChemPhysChem, 2008, 9, 2042-2051. | 2.1 | 32 |
| 39 | Symmetry-adapted perturbation theory interaction energy decomposition for some noble gas complexes. Chemical Physics Letters, 2008, 459, 44-48. | 2.6 | 30 |
| 40 | Predicted NMR properties of noble gas hydride cations RgH+. Chemical Physics Letters, 2008, 467, 18-22. | 2.6 | 11 |
| 41 | Symmetry-Adapted Perturbation-Theory Interaction-Energy Decomposition for Hydrogen-Bonded and Stacking Structures. Journal of Chemical Theory and Computation, 2008, 4, 892-897. | 5.3 | 50 |
| 42 | Microsolvation of HCl within Cold NH<sub>3</sub> Clusters. Journal of Physical Chemistry A, 2008, 112, 11423-11430. | 2.5 | 2 |
| 43 | Interaction in the Ternary Complexes of HClâ‹¯Methanolâ‹¯X, X = H<sub>2</sub>O or NH<sub>3</sub>:â€‰ Ab Initio Calculations and On-the-Fly Molecular Dynamics. Journal of Physical Chemistry A, 2008, 112, 3870-3878. | 2.5 | 3 |
| 44 | Density Functional Theory Study on Vibrational Circular Dichroism as a Tool for Analysis of Intermolecular Systems:â€‰ (1:1) Cysteineâ‹¯Water Complex Conformations. Journal of Physical Chemistry A, 2007, 111, 10703-10711. | 2.5 | 21 |
| 45 | Theoretical Prediction and the First IR Matrix Observation of SeveralL-Cysteine Molecule Conformers. ChemPhysChem, 2007, 8, 1085-1094. | 2.1 | 61 |
| 46 | Cysteine conformations revisited. Computational and Theoretical Chemistry, 2007, 810, 129-134. | 1.5 | 65 |
| 47 | Structure and energetics of weakly bound waterâ€“sulfur dioxide complexes. Computational and Theoretical Chemistry, 2007, 819, 41-51. | 1.5 | 22 |
| 48 | On the calculations of the vibrational Raman spectra of small water clusters. Chemical Physics, 2007, 342, 163-172. | 1.9 | 26 |
| 49 | DFT study of vibrational circular dichroismspectra ofd-lactic acidâ€“water complexes. Physical Chemistry Chemical Physics, 2006, 8, 101-113. | 2.8 | 55 |
| 50 | On the calculations of the nuclear shielding constants in small water clusters. Chemical Physics, 2006, 323, 218-230. | 1.9 | 19 |
| 51 | On the calculations of the nuclear spinâ€“spin coupling constants in small water clusters. Chemical Physics, 2006, 326, 431-444. | 1.9 | 18 |
| 52 | HCl solvation in methanol clusters and nanoparticles: Evidence for proton-wires. Chemical Physics Letters, 2006, 422, 179-183. | 2.6 | 19 |
| 53 | Relativistic calculation of NMR properties of XeF2, XeF4 and XeF6. Chemical Physics Letters, 2006, 427, 281-288. | 2.6 | 37 |
| 54 | Cooperative and anticooperative mixed trimers of HCl and methanol. Journal of Molecular Structure, 2006, 790, 18-26. | 3.6 | 35 |

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|---|---|---|---|
| 55 | HCl Solvation at the Surface and within Methanol Clusters/Nanoparticles II:Â Evidence for Molecular Wires. Journal of Physical Chemistry B, 2006, 110, 21751-21763. | 2.6 | 21 |
| 56 | The Properties of Weak and Strong Dihydrogen-Bonded Dï£¿Hâ‹…â‹…â‹…Hï£¿A Complexes. ChemPhysChem, 2006, 7, 629-639. | 2.1 | 34 |
| 57 | Ab initio study on mixed methanolâ€“hydrogen chloride dimer and trimers. Chemical Physics Letters, 2004, 393, 228-235. | 2.6 | 13 |
| 58 | Solvation Stages of HCl and HBr in Crystalline Phases with Methanol and Small Ethers:Â Acidâˆ'Ether Cluster Complexes in Amorphous and Crystal Phases. Journal of Physical Chemistry A, 2004, 108, 2030-2043. | 2.5 | 20 |
| 59 | Potential Energy and Spinâˆ'Spin Coupling Constants Surface of Glycolaldehyde. Journal of Physical Chemistry A, 2004, 108, 2758-2769. | 2.5 | 18 |
| 60 | The nonadditive effects in the mixed trimers composed of the water dimer and diatomics H2, HF, HCl, HBr, and ClF. Chemical Physics Letters, 2003, 368, 754-768. | 2.6 | 9 |
| 61 | Calculations of hydrogen-bond-transmitted indirect nuclear spinâ€“spin couplings: a comparison of density-functional and ab initio methods. Chemical Physics Letters, 2003, 372, 476-484. | 2.6 | 27 |
| 62 | Characterization of dihydrogen-bonded Dâ€“Hâ‹¯Hâ€“A complexes on the basis of infrared and magnetic resonance spectroscopic parameters. Journal of Chemical Physics, 2003, 119, 5094-5104. | 3.0 | 66 |
| 63 | Ab Initio Calculations of the Intermolecular Nuclear Spin-Spin Coupling Constants. Computational Chemistry - Reviews of Current Trends, 2003, , 131-160. | 0.4 | 4 |
| 64 | Ab initio study of bending modes in water cage clusters, (H2O)n, nï£¾6-10. International Journal of Quantum Chemistry, 2002, 90, 1191-1205. | 2.0 | 16 |
| 65 | Theoretical study of the hydrogen chloride trihydrate. International Journal of Quantum Chemistry, 2002, 90, 1151-1162. | 2.0 | 5 |
| 66 | Ab initio calculations of nonadditive effects in the trimers (H2O)2â‹¯XY,XY=N2, BF, CS. Chemical Physics Letters, 2002, 358, 237-249. | 2.6 | 10 |
| 67 | The spinâ€“spin coupling constants in the ammonia dimer. Chemical Physics Letters, 2002, 360, 272-282. | 2.6 | 15 |
| 68 | Solvation and Ionization Stages of HCl on Ice Nanocrystals. Journal of Physical Chemistry A, 2002, 106, 9374-9389. | 2.5 | 127 |
| 69 | The 19Fâ€“1H coupling constants transmitted through covalent, hydrogen bond, and van der Waals interactions. Journal of Chemical Physics, 2001, 115, 5498-5506. | 3.0 | 43 |
| 70 | Infrared Spectra of Large H2O Clusters:â€‰ New Understanding of the Elusive Bending Mode of Ice. Journal of Physical Chemistry A, 2001, 105, 974-983. | 2.5 | 146 |
| 71 | Reply to the Comment on â€œThe importance of high-order correlation effects for the COâ€“CO interaction potentialâ€•[Chem. Phys. Lett. 314 (1999) 326]. Chemical Physics Letters, 2001, 334, 424-425. | 2.6 | 22 |
| 72 | Benchmark calculations of the shielding constants in the water dimer. Chemical Physics Letters, 2001, 333, 139-145. | 2.6 | 23 |

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|---|---|---|---|
| 73 | The (H2O)2CO ternary complex: cyclic or linear?. Chemical Physics Letters, 2001, 342, 220-230. | 2.6 | 14 |
| 74 | Ab initio study for the intermolecular potential of the waterâ€“nitric oxide complex. Chemical Physics Letters, 2000, 318, 232-239. | 2.6 | 25 |
| 75 | The nuclear spinâ€“spin coupling constants in methanol and methylamine: geometry and solvent effects. Chemical Physics, 2000, 255, 137-148. | 1.9 | 15 |
| 76 | Comprehensive ab initio studies of nuclear magnetic resonance shielding and coupling constants in XHâ‹¯O hydrogen-bonded complexes of simple organic molecules. Journal of Chemical Physics, 2000, 112, 7930-7938. | 3.0 | 49 |
| 77 | Nuclear Magnetic Shielding and Spinâ^'Spin Coupling of 1,2-13C-Enriched Acetylene in Gaseous Mixtures with Xenon and Carbon Dioxide. Journal of Physical Chemistry A, 2000, 104, 5955-5958. | 2.5 | 70 |
| 78 | The Shielding Constants and Scalar Couplings in Nâ^'HÂ·Â·Â·OC and Nâ^'HÂ·Â·Â·NC Hydrogen Bonded Systems:Â An ab Initio MO Study. Journal of Physical Chemistry A, 2000, 104, 8105-8113. | 2.5 | 59 |
| 79 | The asymmetric cage structure of (H2O)7 from a combined spectroscopic and computational study. Journal of Chemical Physics, 1999, 110, 10649-10652. | 3.0 | 113 |
| 80 | The influence of electrostatic and dispersion interactions on the NMR parameters of acetylene. Chemical Physics, 1999, 248, 27-40. | 1.9 | 13 |
| 81 | The geometry dependence of the spinâ€“spin coupling constants in ethane: a theoretical study. Chemical Physics Letters, 1999, 305, 139-146. | 2.6 | 25 |
| 82 | The nuclear spinâ€“spin coupling constants in the water dimer. Chemical Physics Letters, 1999, 308, 486-494. | 2.6 | 37 |
| 83 | The importance of high-order correlation effects for the COâ€“CO interaction potential. Chemical Physics Letters, 1999, 314, 326-332. | 2.6 | 60 |
| 84 | Intermolecular potential of carbon dioxide dimer from symmetry-adapted perturbation theory. Journal of Chemical Physics, 1999, 110, 3785-3803. | 3.0 | 279 |
| 85 | Theoretical Study of Structure and Spectra of Cage Clusters (H2O)n,n= 7â^'10. Journal of Physical Chemistry A, 1999, 103, 4933-4947. | 2.5 | 163 |
| 86 | Solvent effects on NMR spectrum of acetylene calculated by ab initio methods. Chemical Physics, 1998, 234, 111-119. | 1.9 | 49 |
| 87 | Ab initio study of energy, structure and dynamics of the waterâ€“carbon dioxide complex. Journal of Chemical Physics, 1998, 109, 3919-3927. | 3.0 | 51 |
| 88 | Structure and Spectra of Three-Dimensional(H2O)nClusters,n=8,9,10. Physical Review Letters, 1998, 80, 2578-2581. | 7.8 | 309 |
| 89 | Ab initio calculation of and NMR shielding constants in solid acetylene. Solid State Nuclear Magnetic Resonance, 1997, 8, 139-145. | 2.3 | 16 |
| 90 | Abinitiostudy of van der Waals interaction of CO2with Ar. Journal of Chemical Physics, 1996, 104, 6569-6576. | 3.0 | 70 |

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| 91 | Ab initio study of the ground and first excited state of LiAr. International Journal of Quantum Chemistry, 1995, 53, 607-615. | 2.0 | 21 |
| 92 | Ab Initio SCF Calculations Relating to the Cls Chemical Shifts for Some Alkanes. Spectroscopy Letters, 1995, 28, 275-290. | 1.0 | 3 |
| 93 | Ab initiostudy of He(1S)+Cl2(Xâ€‰1Î£g,3Îu) potential energy surfaces. Journal of Chemical Physics, 1994, 101, 6800-6809. | 3.0 | 36 |
| 94 | On the nature of the interaction energy in the Ar-Cl2 complex. Computational and Theoretical Chemistry, 1994, 307, 187-199. | 1.5 | 26 |
| 95 | A study of the weak interaction in SCO/He and SCO/N2 systems. International Journal of Quantum Chemistry, 1993, 46, 623-634. | 2.0 | 18 |
| 96 | Ab initio study of the ground and excited states of LiNe. International Journal of Quantum Chemistry, 1993, 48, 731-741. | 2.0 | 5 |
| 97 | Abinitiostudy of the H2COâ€“Ar complex. Journal of Chemical Physics, 1993, 99, 5211-5218. | 3.0 | 10 |
| 98 | On the nature of the interaction energy in the Arâ€“ClF complex. Journal of Chemical Physics, 1993, 99, 3700-3706. | 3.0 | 24 |
| 99 | Correlatedab initio geometry and vibrational spectra of imidazole and its different forms. International Journal of Quantum Chemistry, 1992, 44, 409-420. | 2.0 | 7 |
| 100 | A quantum chemical study of the hydrogen bonding in a weakly bound SCO-HF complex. Computational and Theoretical Chemistry, 1992, 253, 187-197. | 1.5 | 3 |
| 101 | Ab initio calculations of the vibrational spectra of the ammonia and fluoramide complexes with HF. Computational and Theoretical Chemistry, 1991, 236, 427-441. | 1.5 | 2 |
| 102 | Investigations of the anaesthetic activity of nitrous oxide by quantum-chemical calculations. Computational and Theoretical Chemistry, 1990, 204, 1-14. | 1.5 | 20 |
| 103 | A quantum chemical study of the hydrogen bonding in the CO2?HF and N2O?HF complexes. Theoretica Chimica Acta, 1989, 76, 173-185. | 0.8 | 36 |
| 104 | Ab initio molecular orbital calculations of the IR spectra of hydrogen bonded and lithium bonded complexes of ammonia. Computational and Theoretical Chemistry, 1988, 180, 65-77. | 1.5 | 4 |
| 105 | Ab initio calculations of the vibrational force field and IR intensities of the ammonia dimers. Computational and Theoretical Chemistry, 1987, 150, 223-233. | 1.5 | 3 |
| 106 | Ammonia dimer, linear or cyclic?. Computational and Theoretical Chemistry, 1986, 139, 233-240. | 1.5 | 13 |
| 107 | Spectroscopic parameters of interacting systems. Computational and Theoretical Chemistry, 1982, 88, 71-78. | 1.5 | 9 |
| 108 | An attempt to evaluate the vibrational intensity changes due to long-range interactions. Advances in Molecular Relaxation and Interaction Processes, 1980, 16, 149-154. | 0.5 | 2 |

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| 109 | Spectroscopic parameters of interacting systems. IV.Ab initio study of vibrational band intensity changÃ©s due to ion-molecule interaction in HOHâ€¦Fâ¯. Advances in Molecular Relaxation and Interaction Processes, 1979, 15, 163-172. | 0.5 | 6 |
| 110 | Spectroscopic parameters of interacting systems. V. Ab initio study of vibrational band intensity changes due to hydrogen bonding of the hcnâ€¦hf complex. Advances in Molecular Relaxation and Interaction Processes, 1979, 15, 173-180. | 0.5 | 4 |
| 111 | Theoretical infrared and Raman spectroscopic parameters for H2O and the H2O ? Li+ system. Faraday Discussions of the Chemical Society, 1977, 64, 112. | 2.2 | 22 |
| 112 | The applicability of the CNDO treatment to the interpretation of the infrared spectra of electrolyte solutions in acetone. Human Development, 1973, 5, 253-259. | 0.8 | 2 |
| 113 | Modified CNDO [complete neglect of differential overlap] method. IV. Ion-molecule interactions in the acetone solutions of electrolytes. The Journal of Physical Chemistry, 1971, 75, 3581-3585. | 2.9 | 4 |
| 114 | Properties and Spectroscopies. , 0, , 125-312. | | 3 |