Miroslav Urban

List of Publications by Year
in descending order

20 papers	1,195 citations	933447 10 h-index	794594 19 g-index
21 all docs	21 docs citations	21 times ranked	960 citing authors

#	Article	IF	Citations
1	DFT Functionals for Modeling of Polyethylene Chains Cross-Linked by Metal Atoms. DLPNOâ€“CCSD(T) Benchmark Calculations. Journal of Physical Chemistry A, 2021, 125, 7382-7395.	2.5	8
2	DFT Modeling of Cross-Linked Polyethylene: Role of Gold Atoms and Dispersion Interactions. Journal of Physical Chemistry A, 2018, 122, 1496-1503.	2.5	8
3	Benchmark CCSD(T) and DFT study of binding energies in Be_{7 â^’ 12}: in search of reliable DFT functional for beryllium clusters. Molecular Physics, 2018, 116, 1259-1274.	1.7	9
4	A comparative DFT study of interactions of Au and small gold clusters Aun (n = 2â€“4) with CH3S and CH2 radicals. Chemical Physics Letters, 2017, 671, 84-91.	2.6	8
5	Density functional theory modeling of Câ€“Au chemical bond formation in gold implanted polyethylene. Physical Chemistry Chemical Physics, 2017, 19, 28897-28906.	2.8	12
6	Au_n (n = 1,11) Clusters Interacting With Lone-Pair Ligands. Journal of Physical Chemistry A, 2016, 120, 3938-3949.	2.5	18
7	Toward Understanding the Bonding Character in Complexes of Coinage Metals with Lone-Pair Ligands. CCSD(T) and DFT Computations. Journal of Physical Chemistry A, 2013, 117, 4472-4485.	2.5	34
8	CASPT2 and CCSD(T) calculations of dipole moments and polarizabilities of acetone in excited states. Molecular Physics, 2012, 110, 2219-2237.	1.7	24
9	Highly correlated calculations using optimized virtual orbital space with controlled accuracy. Application to counterpoise corrected interaction energy calculations. International Journal of Quantum Chemistry, 2012, 112, 948-959.	2.0	9
10	Relativistic effects in low-lying electronic states of iron. Theoretical Chemistry Accounts, 2011, 129, 561-566.	1.4	4
11	Relativistic effects in atomic and molecular properties. Acta Physica Slovaca, 2010, 60, .	1.4	58
12	Coreâ€“valence correlation effects in the ground and low-lying excited states of GaN. Molecular Physics, 2010, 108, 467-476.	1.7	0
13	Towards the full coupled-cluster model with triples: a retrospective after 25 years. Molecular Physics, 2010, 108, 2933-2940.	1.7	0
14	Electron affinity of the O₂ molecule: CCSD(T) calculations using the optimized virtual orbitals space approach. International Journal of Quantum Chemistry, 2008, 108, 2159-2171.	2.0	37
15	Theoretical study of molecular properties of low-lying electronic excited states of H₂O and H₂S. Molecular Physics, 2008, 106, 2333-2344.	1.7	30
16	Optimized virtual orbitals for relativistic calculations: an alternative approach to the basis set construction for correlation calculations. Molecular Physics, 2006, 104, 2277-2292.	1.7	34
17	Electric properties of hydrogen iodide: Reexamination of correlation and relativistic effects. Theoretical Chemistry Accounts, 2003, 110, 176-184.	1.4	7
18	Accurate electrical and spectroscopic properties ofX 1?+ BeO from coupled-cluster methods. Theoretica Chimica Acta, 1995, 90, 341-355.	0.8	21

#	Article	IF	Citations
19	On the accuracy of molecular properties by coupled-cluster methods for some difficult examples: Oxygen atom, iron atom, and cyano radical. International Journal of Quantum Chemistry, 1994, 52, 211-225.	2.0	28
20	Towards a full CCSDT model for electron correlation. Journal of Chemical Physics, 1985, 83, 4041-4046.	3.0	843