

# Kushantha P K Withanage

## List of Publications by Year in descending order

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12  
papers

212  
citations

1163117

8  
h-index

1281871

11  
g-index

12  
all docs

12  
docs citations

12  
times ranked

96  
citing authors

#	ARTICLE	IF	CITATIONS
1	Self-consistent self-interaction corrected density functional theory calculations for atoms using Fermi-LÅ¶wdin orbitals: Optimized Fermi-orbital descriptors for Liâ€“Kr. Journal of Chemical Physics, 2017, 147, 164107.	3.0	39
2	Fermi-LÅ¶wdin orbital self-interaction correction to magnetic exchange couplings. Journal of Chemical Physics, 2018, 149, 164101.	3.0	33
3	Shrinking Self-Interaction Errors with the Fermiâ€“LÅ¶wdin Orbital Self-Interaction-Corrected Density Functional Approximation. Journal of Physical Chemistry A, 2018, 122, 9307-9315.	2.5	30
4	The effect of self-interaction error on electrostatic dipoles calculated using density functional theory. Journal of Chemical Physics, 2019, 151, 174106.	3.0	29
5	Self-interaction-free electric dipole polarizabilities for atoms and their ions using the Fermi-LÅ¶wdin self-interaction correction. Physical Review A, 2019, 100, .	2.5	27
6	On the Question of the Total Energy in the Fermiâ€“LÅ¶wdin Orbital Self-Interaction Correction Method. Journal of Chemical Theory and Computation, 2018, 14, 4122-4128.	5.3	22
7	Analytic atomic gradients in the fermiâ€“LÅ¶wdin orbital selfâ€“interaction correction. Journal of Computational Chemistry, 2019, 40, 820-825.	3.3	16
8	Density-related properties from self-interaction corrected density functional theory calculations. Journal of Chemical Physics, 2021, 154, 024102.	3.0	8
9	Complex Fermiâ€“LÅ¶wdin orbital self-interaction correction. Journal of Chemical Physics, 2022, 156, .	3.0	5
10	Fermiâ€“LÅ¶wdin orbital self-interaction correction of adsorption energies on transition metal ions. Journal of Chemical Physics, 2022, 156, 134102.	3.0	2
11	Comment on â€œAdditional Insights Between Fermi-LÅ¶wdin Orbital SIC and the Localization Equation Constraints in SIC-DFTâ€“. Journal of Physical Chemistry A, 2019, 123, 4322-4323.	2.5	1
12	Computational insights into structural and optical properties of P-containing and N-containing ligands capped CdSe clusters. Molecular Simulation, 2019, 45, 1426-1431.	2.0	0