# Kamal Sharkas

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5654835/publications.pdf

Version: 2024-02-01

| 19 | 820 | 516710 | 794594 |
|---|---|---|---|
| papers | citations | 16 | 19 |
| | | h-index | g-index |

| 19 | 19 | 19 | 804 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Double-hybrid density-functional theory made rigorous. Journal of Chemical Physics, 2011, 134, 064113. | 3.0 | 165 |
| 2 | Communication: Rationale for a new class of double-hybrid approximations in density-functional theory. Journal of Chemical Physics, 2011, 135, 101102. | 3.0 | 93 |
| 3 | A multiconfigurational hybrid density-functional theory. Journal of Chemical Physics, 2012, 137, 044104. | 3.0 | 77 |
| 4 | Calculating NMR Chemical Shifts for Paramagnetic Metal Complexes from First-Principles. Journal of Physical Chemistry Letters, 2015, 6, 2183-2188. | 4.6 | 64 |
| 5 | Self-interaction error overbinds water clusters but cancels in structural energy differences. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 11283-11288. | 7.1 | 57 |
| 6 | Ab initio study of the chemical states of water on Cr2O3(0001): From the isolated molecule to saturation coverage. Surface Science, 2009, 603, 2484-2493. | 1.9 | 55 |
| 7 | Analytic Gradients for Complete Active Space Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2018, 14, 126-138. | 5.3 | 40 |
| 8 | Double-hybrid density-functional theory with meta-generalized-gradient approximations. Journal of Chemical Physics, 2014, 140, 084107. | 3.0 | 35 |
| 9 | Fermi-LÃ¶wdin orbital self-interaction correction to magnetic exchange couplings. Journal of Chemical Physics, 2018, 149, 164101. | 3.0 | 33 |
| 10 | Effects from Spinâ€“Orbit Coupling on Electronâ€“Nucleus Hyperfine Coupling Calculated at the Restricted Active Space Level for Kramers Doublets. Journal of Chemical Theory and Computation, 2015, 11, 538-549. | 5.3 | 32 |
| 11 | Shrinking Self-Interaction Errors with the Fermiâ€“LÃ¶wdin Orbital Self-Interaction-Corrected Density Functional Approximation. Journal of Physical Chemistry A, 2018, 122, 9307-9315. | 2.5 | 30 |
| 12 | The effect of self-interaction error on electrostatic dipoles calculated using density functional theory. Journal of Chemical Physics, 2019, 151, 174106. | 3.0 | 29 |
| 13 | Multiconfiguration Pair-Density Functional Theory and Complete Active Space Second Order Perturbation Theory. Bond Dissociation Energies of FeC, NiC, FeS, NiS, FeSe, and NiSe. Journal of Physical Chemistry A, 2017, 121, 9392-9400. | 2.5 | 27 |
| 14 | Double-hybrid density-functional theory applied to molecular crystals. Journal of Chemical Physics, 2014, 141, 044105. | 3.0 | 24 |
| 15 | Range-separated double-hybrid density-functional theory applied to periodic systems. Journal of Chemical Physics, 2015, 143, 102811. | 3.0 | 21 |
| 16 | Towards efficient density functional theory calculations without self-interaction: The Fermi-LÃ¶wdin orbital self-interaction correction. Journal of Physics: Conference Series, 2019, 1290, 012002. | 0.4 | 17 |
| 17 | How well do self-interaction corrections repair the overestimation of static polarizabilities in density functional calculations?. Physical Chemistry Chemical Physics, 2021, 23, 18678-18685. | 2.8 | 14 |
| 18 | The effects of active site and support on hydrogen elimination over transition-metal-functionalized yttria-decorated metalâ€“organic frameworks. Catalysis Science and Technology, 2019, 9, 7003-7015. | 4.1 | 5 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Fermiâ€“LÃ¶wdin orbital self-interaction correction of adsorption energies on transition metal ions. Journal of Chemical Physics, 2022, 156, 134102. | 3.0 | 2 |