Alia V Tadjer

List of Publications by Year
in descending order

34	338	759233 12	839539 18
papers	citations	h-index	g-index

36	36	36	556
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Redox Hyperactive MOF for Li+, Na+ and Mg2+ Storage. Molecules, 2022, 27, 586.	3.8	2
2	Mononuclear copper(II) complexes of the macrolide antibiotics tylosin and tilmicosin. Transition Metal Chemistry, 2022, 47, 67-76.	1.4	2
3	Dinuclear vs. Mononuclear Copper(II) Coordination Species of Tylosin and Tilmicosin in Non-Aqueous Solutions. Molecules, 2022, 27, 3899.	3.8	2
4	Women in the Singlet Fission World: Pearls in a Semi-Open Shell. Molecules, 2021, 26, 2922.	3.8	1
5	Dualâ€Metal Electrolytes for Hybridâ€Ion Batteries: Synergism or Antagonism?. ChemPhysChem, 2021, 22, 1110-1123.	2.1	4
6	The Interplay between Diradical Character and Stability in Organic Molecules. Symmetry, 2021, 13, 1448.	2.2	1
7	Rivalry at the Interface: Ion Desolvation and Electrolyte Degradation in Model Ethylene Carbonate Complexes of Li⁺, Na⁺, and Mg²⁺ with PF₆^{â€“} on the Li₄Ti₅O₁₂ (111) Surface. ACS Omega, 2021, 6, 29735-29745.	3.5	4
8	Topology delimited radicalâ€scavenging propensity of monohydroxycinnamic acids. International Journal of Quantum Chemistry, 2020, 120, e26329.	2.0	1
9	Fundamental promise of anthraquinone functionalized graphene based next generation battery electrodes: a DFT study. Journal of Materials Chemistry A, 2020, 8, 14152-14161.	10.3	11
10	Boron-Doped Polycyclic Aromatic Hydrocarbons: A Molecular Set Revealing the Interplay between Topology and Singlet Fission Propensity. Journal of Physical Chemistry Letters, 2020, 11, 1390-1396.	4.6	21
11	Topology-Dependent Dissociation Mode of the Oâ€“H Bond in Monohydroxycoumarins. Journal of Physical Chemistry A, 2019, 123, 5106-5113.	2.5	6
12	QSAR and molecular docking studies of indole-based analogs as HIV-1 attachment inhibitors. Journal of Molecular Structure, 2019, 1193, 429-443.	3.6	14
13	Insights into the Function of Electrode and Electrolyte Materials in a Hybrid Lithiumâ€“Sodium Ion Cell. Journal of Physical Chemistry C, 2019, 123, 11508-11521.	3.1	16
14	Impacts of hydroxylation on the photophysics of chalcones: insights into the relation between the chemical composition and the electronic structure. Physical Chemistry Chemical Physics, 2018, 20, 8924-8934.	2.8	5
15	In Silico SAR Studies of HIV-1 Inhibitors. Pharmaceuticals, 2018, 11, 69.	3.8	13
16	Density Functional Theory Assessment of the Environment Polarity Effect on Polyanilineâ€“Water Coupling. Journal of Physical Chemistry A, 2017, 121, 6327-6335.	2.5	1
17	Understanding the Fluorescence of TADF Light-Emitting Dyes. Journal of Physical Chemistry A, 2016, 120, 6944-6955.	2.5	26
18	NMR characterization of dilauroyl phosphatidylcholine in adsorbed monolayers at fluid interfaces studied by multiscale computations. International Journal of Quantum Chemistry, 2016, 116, 1419-1426.	2.0	5

#	Article	IF	Citations
19	Fully atomistic molecularâ€mechanical model of liquid alkane oils: Computational validation. Journal of Computational Chemistry, 2014, 35, 776-788.	3.3	6
20	Magnetostructural Correlation for Rational Design of Mn(II) Hybrid-Spin Complexes. Journal of Physical Chemistry A, 2013, 117, 670-678.	2.5	2
21	Absorption Spectra of Model Single Chains of Conducting Polyaniline. Journal of Physical Chemistry B, 2012, 116, 6543-6552.	2.6	14
22	Fully Doped Oligomers of Emeraldine Salt: Polaronic versus Bipolaronic Configuration. Journal of Physical Chemistry B, 2011, 115, 3765-3776.	2.6	21
23	Solvent polarity and dopant effect on the electronic structure of the emeraldine salt. International Journal of Quantum Chemistry, 2011, 111, 435-443.	2.0	17
24	Theoretical Study on the Structural Aspects of CuIIHybrid-Spin Complexes. European Journal of Inorganic Chemistry, 2010, 2010, 379-390.	2.0	4
25	Theoretical study on the emeraldine salt â€“ impact of the computational protocol. Computational and Theoretical Chemistry, 2010, 954, 36-44.	1.5	25
26	Systematic theoretical study of Li adsorption on stable BN- and B-substituted aromatic hydrocarbons. Computational and Theoretical Chemistry, 2010, 955, 109-122.	1.5	7
27	Boronâ€“nitrogen- and boron-substituted anthracenes and -phenanthrenes as models for doped carbon-based materials. Computational and Theoretical Chemistry, 2010, 955, 97-108.	1.5	7
28	Unprecedented Route to Ordered Polyaniline: Direct Synthesis of Highly Crystalline Fibrillar Films with Strong Ï€â€¿Ï€ Stacking Alignment. Macromolecular Rapid Communications, 2009, 30, 29-33.	3.9	42
29	Influence of the Level of Protonation on the Geometry and the Electronic Structure of Emeraldine Oligomers. Progress in Theoretical Chemistry and Physics, 2009, , 219-251.	0.2	1
30	Anticancer Activity of Spin-Labeled Nitrosoureas as a Function of the LUMO Energy. , 2008, , .		0
31	Evidence for Generation of Delocalized Polarons in Conducting Polyaniline: A Raman Scattering Spectroscopy Approach. International Journal of Polymer Analysis and Characterization, 2007, 12, 251-271.	1.9	23
32	Radical scavenging activity prediction of o-coumaric acid thioamide. Computational and Theoretical Chemistry, 2007, 821, 133-138.	1.5	13
33	First principle study of the structure of conjugated amides and thioamides. International Journal of Quantum Chemistry, 2007, 107, 1765-1771.	2.0	8
34	Theoretical Study of the Influence of Monomer Excess on the Structure and Properties of Polyaniline Oligomers. Journal of Physical Chemistry B, 2006, 110, 2555-2564.	2.6	13