Esam A Orabi

List of Publications by Year in Descending Order

30 papers	422 citations	13 h-index	19 g-index
30 ext. papers	516 ext. citations	4.7 avg, IF	4.57 L-index

#	Paper	IF	Citations
30	Inter/intramolecular hydrogen bonding mediate miscible blend formation between near-perfect alternating Poly(styrene-alt- hydroxyphenylmaleimide) copolymers and Poly(vinyl pyrrolidone). *Polymer*, **2021**, 219, 123542	3.9	7
29	Twisted Intramolecular Charge Transfer (TICT) Controlled by Dimerization: An Overlooked Piece of the TICT Puzzle. *Journal of Physical Chemistry A*, **2021**, 125, 2885-2894	2.8	6
28	Molecular dynamics investigation of the structural flexibility of H2O2 and H2S2 in response to medium polarity. *Journal of Molecular Liquids*, **2021**, 329, 115469	6	1
27	Modeling Shows that Rotation about the Peroxide O-O Bond Assists Protein and Lipid Functional Groups in Discriminating between HO and HO. *Journal of Physical Chemistry B*, **2021**, 125, 137-147	3.4	2
26	Corrections in the CHARMM36 Parametrization of Chloride Interactions with Proteins, Lipids, and Alkali Cations, and Extension to Other Halide Anions. *Journal of Chemical Theory and Computation*, **2021**, 17, 6240-6261	6.4	0
25	Biologically-Active Heterocyclic Molecules with Aggregation-Induced Blue-Shifted Emission and Efficient Luminescence both in Solution and Solid States. *Journal of Photochemistry and Photobiology A: Chemistry*, **2020**, 400, 112642	4.7	13
24	New Molecular-Mechanics Model for Simulations of Hydrogen Fluoride in Chemistry and Biology. *Journal of Chemical Theory and Computation*, **2020**, 16, 5105-5126	6.4	10
23	Aggregation-induced emission with white, green, or blue luminescence from biologically-active indole derivatives. *Optical Materials*, **2020**, 100, 109713	3.3	12
22	Drude polarizable force field for cation-interactions of alkali and quaternary ammonium ions with aromatic amino acid side chains. *Journal of Computational Chemistry*, **2020**, 41, 472-481	3.5	7
21	Synthesis of Novel Biocompatible Thienopyrimidine Chromophores with Aggregation-Induced Emission Sensitive to Molecular Aggregation. *ACS Omega*, **2020**, 5, 29988-30000	3.9	8
20	Structures, NMR Spectroscopic Features, and Cytotoxic Properties of Oligomeric Hellinoyl (-GO--GOG)-Type Ellagitannins from the Galls of. *Journal of Natural Products*, **2019**, 82, 2682-2695	4.9	0
19	Expanding the range of binding energies and oxidizability of biologically relevant S-aromatic interactions: imidazolium and phenolate binding to sulfoxide and sulfone. *Physical Chemistry Chemical Physics*, **2019**, 21, 14620-14628	3.6	5
18	Computational insight into hydrogen persulfide and a new additive model for chemical and biological simulations. *Physical Chemistry Chemical Physics*, **2019**, 21, 15988-16004	3.6	6
17	Conducting copolymers nanocomposite coatings with aggregation-controlled luminescence and efficient corrosion inhibition properties. *Progress in Organic Coatings*, **2019**, 135, 525-535	4.8	18
16	A Simple Additive Potential Model for Simulating Hydrogen Peroxide in Chemical and Biological Systems. *Journal of Chemical Theory and Computation*, **2018**, 14, 2808-2821	6.4	12
15	Cation-Interactions between Quaternary Ammonium Ions and Amino Acid Aromatic Groups in Aqueous Solution. *Journal of Physical Chemistry B*, **2018**, 122, 2251-2260	3.4	19
14	Computational investigation of the structure and antioxidant activity of some pyrazole and pyrazolone derivatives. *Journal of Saudi Chemical Society*, **2018**, 22, 705-714	4.3	19

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13	Modeling Protein S-Aromatic Motifs Reveals Their Structural and Redox Flexibility. *Journal of Physical Chemistry B*, **2018**, 122, 3760-3770	3.4	18
12	Predicting structural and energetic changes in Met-aromatic motifs on methionine oxidation to the sulfoxide and sulfone. *Physical Chemistry Chemical Physics*, **2018**, 20, 23132-23141	3.6	10
11	Tautomerism and antioxidant activity of some 4-acylpyrazolone-based Schiff bases: a theoretical study.. *RSC Advances*, **2018**, 8, 30842-30850	3.7	15
10	Sulfur-Aromatic Interactions: Modeling Cysteine and Methionine Binding to Tyrosinate and Histidinium Ions to Assess Their Influence on Protein Electron Transfer. *Israel Journal of Chemistry*, **2016**, 56, 872-885	3.4	20
9	Mechanism of NH4(+) Recruitment and NH3 Transport in Rh Proteins. *Structure*, **2015**, 23, 1550-1557	5.2	21
8	Simulation of Liquid and Supercritical Hydrogen Sulfide and of Alkali Ions in the Pure and Aqueous Liquid. *Journal of Chemical Theory and Computation*, **2014**, 10, 3221-35	6.4	15
7	Polarizable Interaction Model for Liquid, Supercritical, and Aqueous Ammonia. *Journal of Chemical Theory and Computation*, **2013**, 9, 2035-51	6.4	17
6	Molecular Dynamics Investigation of Alkali Metal Ions in Liquid and Aqueous Ammonia. *Journal of Chemical Theory and Computation*, **2013**, 9, 2324-38	6.4	23
5	Molecular modelling of cation interactions. *Molecular Simulation*, **2012**, 38, 704-722	2	20
4	Cation- and Interactions in Aqueous Solution Studied Using Polarizable Potential Models. *Journal of Chemical Theory and Computation*, **2012**, 8, 182-93	6.4	58
3	Ammonium transporters achieve charge transfer by fragmenting their substrate. *Journal of the American Chemical Society*, **2012**, 134, 10419-27	16.4	54
2	Theoretical study of inner and outer mononuclear complexes of Co(II), Ni(II), and Cu(II) with a compartmental hexadentate Schiff base derived from 3-formylsalicylic acid. *Journal of Coordination Chemistry*, **2010**, 63, 4017-4029	1.6	2
1	Spectroscopic studies on 3- and 5-formylsalicylic acids and their complexes with Fe(III). *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2010**, 75, 918-24	4.4	4