Emilie B Guidez

List of Publications by Year
in descending order

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23 papers	1,385 citations	623734 14 h-index	642732 23 g-index
23 all docs	23 docs citations	23 times ranked	1720 citing authors

#	Article	IF	Citations
1	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	3.0	734
2	Effects of Silver Doping on the Geometric and Electronic Structure and Optical Absorption Spectra of the Au_{25â€“n}Ag_n(SH)₁₈^{â€“} (n = 1,) TJETQq0 0 0 rgBT /Ov	3	0
3	Quantum mechanical origin of the plasmon: from molecular systems to nanoparticles. Nanoscale, 2014, 6, 11512-11527.	5.6	97
4	Theoretical analysis of the optical excitation spectra of silver and gold nanowires. Nanoscale, 2012, 4, 4190.	5.6	81
5	Quantum coherent plasmon in silver nanowires: A real-time TDDFT study. Journal of Chemical Physics, 2014, 140, 244705.	3.0	57
6	Photoluminescence Origin of Au38(SR)24 and Au22(SR)18 Nanoparticles: A Theoretical Perspective. Journal of Physical Chemistry C, 2017, 121, 15416-15423.	3.1	53
7	Perspective: Ab initio force field methods derived from quantum mechanics. Journal of Chemical Physics, 2018, 148, .	3.0	52
8	Theoretical Investigation of Relaxation Dynamics in Au₃₈(SH)₂₄ Thiolate-Protected Gold Nanoclusters. Journal of Physical Chemistry C, 2018, 122, 16380-16388.	3.1	27
9	Plasmon resonance analysis with configuration interaction. Physical Chemistry Chemical Physics, 2014, 16, 15501.	2.8	24
10	Why is Si₂H₂ Not Linear? An Intrinsic Quasi-Atomic Bonding Analysis. Journal of the American Chemical Society, 2020, 142, 13729-13742.	13.7	19
11	Derivation and Implementation of the Gradient of the R^{â€“7} Dispersion Interaction in the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2016, 120, 639-647.	2.5	18
12	Dispersion Correction Derived from First Principles for Density Functional Theory and Hartreeâ€“Fock Theory. Journal of Physical Chemistry A, 2015, 119, 2161-2168.	2.5	17
13	Synthesis and Characterization of Gallium-Doped CdSe Quantum Dots. Journal of Physical Chemistry C, 2015, 119, 10749-10757.	3.1	17
14	Time-Dependent Density Functional Theory Study of the Luminescence Properties of Gold Phosphine Thiolate Complexes. Journal of Physical Chemistry A, 2015, 119, 3337-3347.	2.5	14
15	Development of a charge-perturbed particle-in-a-sphere model for nanoparticle electronic structure. Physical Chemistry Chemical Physics, 2012, 14, 4287.	2.8	12
16	Traversing the Tightrope between Halogen and Chalcogen Bonds Using Structural Chemistry and Theory. Crystal Growth and Design, 2021, 21, 7168-7178.	3.0	12
17	Dispersion Interactions in Water Clusters. Journal of Physical Chemistry A, 2017, 121, 3736-3745.	2.5	10
18	Accuracy of the PM6 and PM7 Methods on Bare and Thiolate-Protected Gold Nanoclusters. Journal of Physical Chemistry A, 2020, 124, 2601-2615.	2.5	8

#	Article	IF	Citations
19	Quantum Mechanical Modeling of the Interactions between Noble Metal (Ag and Au) Nanoclusters and Water with the Effective Fragment Potential Method. ACS Omega, 2020, 5, 7446-7455.	3.5	7
20	Adaptive-Partitioning Multilayer Dynamics Simulations: 1. On-the-Fly Switch between Two Quantum Levels of Theory. Journal of Chemical Theory and Computation, 2021, 17, 5456-5465.	5.3	7
21	Computation of hostâ€“guest binding free energies with a new quantum mechanics based mining minima algorithm. Journal of Chemical Physics, 2021, 154, 104122.	3.0	6
22	Benchmarking the Effective Fragment Potential Dispersion Correction on the S22 Test Set. Journal of Physical Chemistry A, 2018, 122, 4076-4084.	2.5	3
23	Benchmarking of the R^{â€“7} Anisotropic Dispersion Energy Term on the S22 Dimer Test Set. Journal of Physical Chemistry A, 2018, 122, 6100-6108.	2.5	2