

# Emilie B Guidez

## List of Publications by Year in descending order

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Version: 2024-02-01

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	Computation of host-guest binding free energies with a new quantum mechanics based mining minima algorithm. <i>Journal of Chemical Physics</i> , 2021, 154, 104122.	3.0	6
2	Adaptive-Partitioning Multilayer Dynamics Simulations: 1. On-the-Fly Switch between Two Quantum Levels of Theory. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5456-5465.	5.3	7
3	Traversing the Tightrope between Halogen and Chalcogen Bonds Using Structural Chemistry and Theory. <i>Crystal Growth and Design</i> , 2021, 21, 7168-7178.	3.0	12
4	Why is Si <sub>2</sub> H <sub>2</sub> Not Linear? An Intrinsic Quasi-Atomic Bonding Analysis. <i>Journal of the American Chemical Society</i> , 2020, 142, 13729-13742.	13.7	19
5	Accuracy of the PM6 and PM7 Methods on Bare and Thiolate-Protected Gold Nanoclusters. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2601-2615.	2.5	8
6	Quantum Mechanical Modeling of the Interactions between Noble Metal (Ag and Au) Nanoclusters and Water with the Effective Fragment Potential Method. <i>ACS Omega</i> , 2020, 5, 7446-7455.	3.5	7
7	Recent developments in the general atomic and molecular electronic structure system. <i>Journal of Chemical Physics</i> , 2020, 152, 154102.	3.0	734
8	Benchmarking the Effective Fragment Potential Dispersion Correction on the S22 Test Set. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4076-4084.	2.5	3
9	Perspective: <i>Ab initio</i> force field methods derived from quantum mechanics. <i>Journal of Chemical Physics</i> , 2018, 148, .	3.0	52
10	Benchmarking of the <i>R<sup>7</sup></i> Anisotropic Dispersion Energy Term on the S22 Dimer Test Set. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6100-6108.	2.5	2
11	Theoretical Investigation of Relaxation Dynamics in Au <sub>38</sub> (SH) <sub>24</sub> Thiolate-Protected Gold Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2018, 122, 16380-16388.	3.1	27
12	Dispersion Interactions in Water Clusters. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3736-3745.	2.5	10
13	Photoluminescence Origin of Au <sub>38</sub> (SR) <sub>24</sub> and Au <sub>22</sub> (SR) <sub>18</sub> Nanoparticles: A Theoretical Perspective. <i>Journal of Physical Chemistry C</i> , 2017, 121, 15416-15423.	3.1	53
14	Derivation and Implementation of the Gradient of the <i>R<sup>7</sup></i> Dispersion Interaction in the Effective Fragment Potential Method. <i>Journal of Physical Chemistry A</i> , 2016, 120, 639-647.	2.5	18
15	Time-Dependent Density Functional Theory Study of the Luminescence Properties of Gold Phosphine Thiolate Complexes. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3337-3347.	2.5	14
16	Dispersion Correction Derived from First Principles for Density Functional Theory and Hartree-Fock Theory. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2161-2168.	2.5	17
17	Synthesis and Characterization of Gallium-Doped CdSe Quantum Dots. <i>Journal of Physical Chemistry C</i> , 2015, 119, 10749-10757.	3.1	17
18	Quantum coherent plasmon in silver nanowires: A real-time TDDFT study. <i>Journal of Chemical Physics</i> , 2014, 140, 244705.	3.0	57

#	ARTICLE	IF	CITATIONS
19	Quantum mechanical origin of the plasmon: from molecular systems to nanoparticles. <i>Nanoscale</i> , 2014, 6, 11512-11527.	5.6	97
20	Plasmon resonance analysis with configuration interaction. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 15501.	2.8	24
21	Development of a charge-perturbed particle-in-a-sphere model for nanoparticle electronic structure. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 4287.	2.8	12
22	Effects of Silver Doping on the Geometric and Electronic Structure and Optical Absorption Spectra of the Au <sub>25</sub> Ag <sub>18</sub> (SH) <sub>18</sub> <sup>+</sup> (n = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100) <i>JETQ 0.0 BT / Over</i>	1.0	0
23	Theoretical analysis of the optical excitation spectra of silver and gold nanowires. <i>Nanoscale</i> , 2012, 4, 4190.	5.6	81