Javier Hernandez-Rojas

List of Publications by Year
in descending order

53	1,166	394421	414414
papers	citations	19 h-index	32 g-index

53	53	53	1046
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Global minima for water clusters (H2O)n, nâ©½21, described by a five-site empirical potential. Chemical Physics Letters, 2005, 415, 302-307.	2.6	148
2	Crystals of binary Lennard-Jones solids. Physical Review B, 2001, 64, .	3.2	77
3	Global Potential Energy Minima of C60(H2O)n Clusters. Journal of Physical Chemistry B, 2006, 110, 13357-13362.	2.6	55
4	Global minima and energetics of Li+(H2O)n and Ca2+(H2O)n clusters for nâ©½20. Chemical Physics Letters, 2005, 412, 23-28.	2.6	53
5	Global minima for rare gas clusters containing one alkali metal ion. Journal of Chemical Physics, 2003, 119, 7800-7804.	3.0	51
6	Confinement Effects on Water Clusters Inside Carbon Nanotubes. Journal of Physical Chemistry C, 2012, 116, 17019-17028.	3.1	48
7	Energy landscapes for shells assembled from pentagonal and hexagonal pyramids. Physical Chemistry Chemical Physics, 2009, 11, 2098.	2.8	44
8	Global Potential Energy Minima of (H₂O)_n Clusters on Graphite. Journal of Physical Chemistry C, 2007, 111, 14862-14869.	3.1	33
9	Microcanonical versus Canonical Analysis of Protein Folding. Physical Review Letters, 2008, 100, 258104.	7.8	33
10	Rotational spectra for offâ€center endohedral atoms at C60 fullerene. Journal of Chemical Physics, 1996, 104, 1179-1186.	3.0	31
11	Modeling Water Clusters on Cationic Carbonaceous Seeds. Journal of Physical Chemistry A, 2010, 114, 7267-7274.	2.5	31
12	Thermodynamics of water octamer in a uniform electric field. Journal of Chemical Physics, 2006, 125, 224302.	3.0	30
13	Coronene molecules in helium clusters: Quantum and classical studies of energies and configurations. Journal of Chemical Physics, 2015, 143, 224306.	3.0	28
14	Lithium ions solvated in helium. Physical Chemistry Chemical Physics, 2018, 20, 25569-25576.	2.8	25
15	Coarse-graining the structure of polycyclic aromatic hydrocarbons clusters. Physical Chemistry Chemical Physics, 2016, 18, 13736-13740.	2.8	23
16	Optimal covering of C60 fullerene by rare gases. Journal of Chemical Physics, 2012, 137, 074306.	3.0	22
17	Adsorption of molecular hydrogen on coronene with a new potential energy surface. Physical Chemistry Chemical Physics, 2017, 19, 26358-26368.	2.8	22
18	Lowest-energy structures of (C[sub 60])[sub n]X (X=Li[sup +],Na[sup +],K[sup +],Cl[sup â^']) and (C[sub) Tj ETQq0 0 0 rgBT /Overlock	3.0	21

#	Article	IF	Citations
19	Physical properties of small water clusters in low and moderate electric fields. Journal of Chemical Physics, 2011, 135, 124303.	3.0	19
20	Polarization effects in C60 fullerene complexes of alkali ions. Journal of Chemical Physics, 1998, 109, 3573-3579.	3.0	17
21	Water clusters confined in icosahedral fullerene cavities. Chemical Physics, 2012, 399, 240-244.	1.9	17
22	The effect of dispersion damping functions on the structure of water clusters. Chemical Physics, 2014, 444, 23-29.	1.9	17
23	Self-assembly of colloidal magnetic particles: energy landscapes and structural transitions. Physical Chemistry Chemical Physics, 2016, 18, 26579-26585.	2.8	17
24	Dynamics and thermodynamics of the coronene octamer described by coarse-grained potentials. Physical Chemistry Chemical Physics, 2017, 19, 1884-1895.	2.8	17
25	A combined experimental and theoretical investigation of Cs+ ions solvated in HeN clusters. Journal of Chemical Physics, 2019, 150, 154304.	3.0	17
26	Examination of the Feynmanâ€“Hibbs Approach in the Study of Ne_N-Coronene Clusters at Low Temperatures. Journal of Physical Chemistry A, 2016, 120, 5370-5379.	2.5	16
27	Comparative investigation of pure and mixed rare gas atoms on coronene molecules. Journal of Chemical Physics, 2017, 146, 034302.	3.0	16
28	On polarization effects in endohedral fullerene complexes. Chemical Physics Letters, 1995, 235, 160-162.	2.6	15
29	Rotational dynamics of endohedral C60 fullerene complexes. Journal of Physics and Chemistry of Solids, 1997, 58, 1689-1696.	4.0	15
30	Global minima of (C60)nCa2+, (C60)nFâ¯ and (C60)nIâ¯ clusters. Chemical Physics Letters, 2005, 410, 404-409.	2.6	15
31	A semi-empirical analytical potential for diatomic molecules at spherical fullerenes. Chemical Physics Letters, 1994, 222, 88-94.	2.6	14
32	Supercooled Lennard-Jones liquids and glasses: a kinetic Monte Carlo approach. Journal of Non-Crystalline Solids, 2004, 336, 218-222.	3.1	14
33	A minimal representation of the self-assembly of virus capsids. Soft Matter, 2014, 10, 3560.	2.7	14
34	Free and hindered rotations in endohedral C60 fullerene complexes. International Journal of Quantum Chemistry, 1997, 65, 655-663.	2.0	13
35	Low-temperature dynamics and spectroscopy in exohedral rare-gas C60 fullerene complexes. Journal of Chemical Physics, 2001, 114, 5156-5163.	3.0	12
36	Applicability of Quantum Thermal Baths to Complex Many-Body Systems with Various Degrees of Anharmonicity. Journal of Chemical Theory and Computation, 2015, 11, 861-870.	5.3	12

#	Article	IF	Citations
37	Snowball formation for Cs⁺ solvation in molecular hydrogen and deuterium. Physical Chemistry Chemical Physics, 2019, 21, 15662-15668.	2.8	12
38	On the rotational spectra of endohedral atoms at fullerenes: the off-centre case. Chemical Physics Letters, 1995, 237, 115-122.	2.6	11
39	Kinetics of empty viral capsid assembly in a minimal model. Soft Matter, 2019, 15, 7166-7172.	2.7	11
40	Coarse-grained modeling of the nucleation of polycyclic aromatic hydrocarbons into soot precursors. Physical Chemistry Chemical Physics, 2019, 21, 5123-5132.	2.8	10
41	On polarization effects in endohedral fullerene complexes (Chem. Phys. Letters 235 (1995) 160). Chemical Physics Letters, 1995, 243, 587-588.	2.6	9
42	Global Potential Energy Minima of (H₂O)_nClusters on Graphite: A Comparative Study of the TIPNP (N= 3, 4, 5) Family. Journal of Physical Chemistry C, 2008, 112, 16497-16504.	3.1	9
43	Raman rotational spectra of endohedral C60 fullerene complexes. Journal of Chemical Physics, 1996, 105, 4482-4487.	3.0	8
44	Minimal Design Principles for Icosahedral Virus Capsids. ACS Nano, 2021, 15, 14873-14884.	14.6	8
45	Caging effects in the lowâ€temperature rotational spectra of endohedral diatomic molecules at C60 fullerene. Journal of Chemical Physics, 1996, 104, 5754-5760.	3.0	6
46	Density effects in a bulk binary Lennard-Jones system. Physical Review B, 2003, 68, .	3.2	6
47	Ca+ Ions Solvated in Helium Clusters. Molecules, 2021, 26, 3642.	3.8	6
48	Temperature- and field-induced structural transitions in magnetic colloidal clusters. Physical Review E, 2018, 97, 022601.	2.1	5
49	Growth of rare gases on coronene. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	5
50	A minimal coarse-grained model for the low-frequency normal mode analysis of icosahedral viral capsids. Soft Matter, 2020, 16, 3443-3455.	2.7	4
51	The Structure of Adamantane Clusters: Atomistic vs. Coarse-Grained Predictions From Global Optimization. Frontiers in Chemistry, 2019, 7, 573.	3.6	3
52	Rare gas-naphthalene interaction: Intermolecular potentials and clustersâ€™ structures. Chemical Physics Letters, 2021, 773, 138565.	2.6	1
53	Energy landscapes and dynamics of polycyclic aromatic hydrocarbon clusters from coarse-grained models. Frontiers of Nanoscience, 2022, , 19-41.	0.6	0