Celine Leonard

List of Publications by Year
in descending order

71 papers	1,161 citations	516710 16 h-index	434195 31 g-index
71 all docs	71 docs citations	71 times ranked	927 citing authors

#	Article	IF	Citations
1	Calculation and selective population of vibrational levels with the Multiconfiguration Time-Dependent Hartree (MCTDH) algorithm. Chemical Physics, 2006, 329, 179-192.	1.9	215
2	Tuning the band gap and optical spectra of silicon-doped graphene: Many-body effects and excitonic states. Journal of Alloys and Compounds, 2017, 693, 1185-1196.	5.5	119
3	Quasi-particle energies and optical excitations of wurtzite BeO and its nanosheet. Journal of Alloys and Compounds, 2016, 682, 254-262.	5.5	63
4	The vibrational levels of ammonia. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 825-838.	3.9	62
5	Time-dependent wave packet study ontrans-cisisomerization of HONO driven by an external field. Journal of Chemical Physics, 2007, 127, 164315.	3.0	47
6	The barrier to inversion of ammonia. Chemical Physics Letters, 2003, 370, 360-365.	2.6	43
7	Potential Energy Function and Vibrational States of the Electronic Ground State of N4+. Journal of Physical Chemistry A, 1999, 103, 1846-1852.	2.5	37
8	Potential energy function and vibrational states of N2CO+. Journal of Chemical Physics, 1999, 111, 4948-4955.	3.0	29
9	Rovibrational energy levels of the F^{â^'}(H₂O) and F^{â^'}(D₂O) complexes. Physical Chemistry Chemical Physics, 2016, 18, 17678-17690.	2.8	22
10	New study of the stability and of the spectroscopy of the molecular anions NCOâ^' and CNOâ^'. Journal of Chemical Physics, 2010, 133, 124318.	3.0	21
11	The selective population of the vibrational levels of thioformaldehyde. Physical Chemistry Chemical Physics, 2001, 3, 508-513.	2.8	20
12	Theoretical investigation of intramolecular vibrational energy redistribution in HFCO and DFCO induced by an external field. Journal of Chemical Physics, 2008, 129, 144304.	3.0	18
13	Rennerâ€"Teller effect in linear tetra-atomic molecules. I. Variational method including couplings between all degrees of freedom on six-dimensional potential energy surfaces. Journal of Chemical Physics, 2009, 130, 134301.	3.0	18
14	Argon Interaction with Gold Surfaces: Ab Initio-Assisted Determination of Pair Arâ€"Au Potentials for Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2015, 119, 6897-6908.	2.5	18
15	Ab initio study of the low-lying electronic states of the CaO molecule. Chemical Physics, 2011, 386, 50-55.	1.9	17
16	Effects of surface morphology and anisotropy on the tangential-momentum accommodation coefficient between Pt(100) and Ar. Physical Review E, 2012, 86, 051201.	2.1	17
17	Free-path distribution and Knudsen-layer modeling for gaseous flows in the transition regime. Physical Review E, 2015, 91, 023015.	2.1	17
18	Rennerâ€"Teller effect in linear tetra-atomic molecules. II. Rovibronic levels analysis of the Xâ€‰Î2u electronic state of HCCH+. Journal of Chemical Physics, 2009, 130, 134302.	3.0	16

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19	Selective vibrational excitations in the OX (X=F, Cl, Br, I) molecules. Physical Chemistry Chemical Physics, 2000, 2, 1117-1122.	2.8	15
20	A slip model for micro/nano gas flows induced by body forces. Microfluidics and Nanofluidics, 2010, 8, 417-422.	2.2	15
21	Theoretical Study of the Rovibronic States of CaO. Journal of Molecular Spectroscopy, 2012, 271, 1-9.	1.2	14
22	Non-parametric wall model and methods of identifying boundary conditions for moments in gas flow equations. Physics of Fluids, 2018, 30, .	4.0	14
23	Prediction of thermal conductance and friction coefficients at a solid-gas interface from statistical learning of collisions. Physical Review E, 2018, 98, .	2.1	13
24	Influence of the pairwise potential on the tangential momentum accommodation coefficient: a multi-scale study applied to the argon on Pt(111) system. European Physical Journal B, 2013, 86, 1.	1.5	12
25	Bound electronic states X1Î£+, a3Î and A1Î of C2B-. Physical Chemistry Chemical Physics, 1999, 1, 1827-1832.	2.8	11
26	Theoretical determination of the vibrational levels of NH+3and its isotopomers. Molecular Physics, 2001, 99, 1335-1346.	1.7	11
27	Theoretical enthalpies of formation of large compounds using integrated methods. Physical Chemistry Chemical Physics, 2002, 4, 4096-4102.	2.8	11
28	Spinâ€“orbit coupling in the X2Î state of NCS. Chemical Physics Letters, 2004, 398, 123-129.	2.6	11
29	New Variational Method for the Ab Initio Study in Valence Coordinates of the Rennerâ^'Teller Effect in Tetra-Atomic Systems. Journal of Chemical Theory and Computation, 2010, 6, 1565-1579.	5.3	11
30	Non-covalent functionalization of single walled carbon nanotubes with Fe-/Co-porphyrin and Co-phthalocyanine for field-effect transistor applications. Organic Electronics, 2021, 96, 106212.	2.6	11
31	Molecular Dynamics Simulations of Pressure-Driven Flows and Comparison with Acceleration-Driven Flows. Advances in Mechanical Engineering, 2012, 4, 580763.	1.6	11
32	Theoretical determination of the vibrational levels of NH3+with MULTIMODE. Physical Chemistry Chemical Physics, 2002, 4, 4087-4095.	2.8	10
33	Ab initio study of the spectroscopy of the X2Î electronic ground states of CNO and NCO. Journal of Molecular Spectroscopy, 2007, 243, 90-98.	1.2	10
34	Theoretical Investigations on CaO Ions: Vibronic States and Photoelectron Spectroscopy. Journal of Physical Chemistry A, 2013, 117, 11254-11260.	2.5	10
35	A theoretical spectroscopic study of HeI and HeBr. Physical Chemistry Chemical Physics, 2005, 7, 1694-1699.	2.8	9
36	Radiative transition probabilities in the state of. Journal of Quantitative Spectroscopy and Radiative Transfer, 2008, 109, 535-548.	2.3	9

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37	Electronic States, Potential Energy Surface, and Theoretical Spectroscopy of Be₂H₂. Journal of Physical Chemistry A, 2012, 116, 9484-9489.	2.5	9
38	Wet-Chemical Noncovalent Functionalization of CVD Graphene: Molecular Doping and Its Effect on Electrolyte-Gated Graphene Field-Effect Transistor Characteristics. Journal of Physical Chemistry C, 2022, 126, 4522-4533.	3.1	9
39	Large amplitude vibrations in the Xâ€Š[sup 2]A[sub 1] state of C[sub 2]B. Journal of Chemical Physics, 2000, 113, 5228.	3.0	8
40	Ab initiostudy of the low lying electronic states of ZnF and ZnFâ^'. Journal of Chemical Physics, 2008, 129, 044313.	3.0	8
41	Boundary conditions for gas flow problems from anisotropic scattering kernels. Journal of Mathematical Physics, 2015, 56, .	1.1	8
42	Spin-dependent and Coriolis interactions by an improved configuration interaction treatment: predissociation of excited fine structure levels of OH/OD. Molecular Physics, 2000, 98, 1713-1727.	1.7	7
43	Ab initio study of the first excited state <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si240.gif" display="inline" overflow="scroll"><mml:mrow><mml:msup><mml:mrow><mml:mtext>A</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msup></mml:mrow><mml:mrow><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:mrow></mml:math> and of the transition <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si241.gif" di. Chemical Physics Letters, 2008, 458, 24-28.	2.0	7
44	CCSD(T)â€F12 investigations on HBNH and its isotopologues. International Journal of Quantum Chemistry, 2012, 112, 2051-2061.	2.0	7
45	Helium and Argon Interactions with Gold Surfaces: Ab Initio-Assisted Determination of the Heâ€“Au Pairwise Potential and Its Application to Accommodation Coefficient Determination. Journal of Physical Chemistry C, 2018, 122, 14606-14614.	3.1	7
46	Mg2H2: New insight on the Mgâ€“Mg bonding and spectroscopic study. Journal of Chemical Physics, 2011, 134, 054314.	3.0	6
47	Study of the $ilde{m X}^2Pi$XÌƒ2Î state of the SiCN/SiNC Renner-Teller system. Journal of Chemical Physics, 2013, 138, 104311.	3.0	6
48	Tensorial slip theory for gas flows and comparison with molecular dynamics simulations using an anisotropic gas-wall collision mechanism. Physical Review E, 2013, 87, 053012.	2.1	6
49	Theoretical study of the Aâ€“X transition in C2Bâ^'. Chemical Physics, 2001, 264, 267-273.	1.9	5
50	Ab initiostudy of the spinâ€“orbit coupling between the A and b3Îuelectronic states of Na2. Molecular Physics, 2007, 105, 1095-1104.	1.7	5
51	Theoretical spectroscopy of the HNClâ^' anion. Molecular Physics, 2011, 109, 2655-2662.	1.7	5
52	Rovibrational energies of B2H2() from an explicitly correlated potential energy surface. Computational and Theoretical Chemistry, 2013, 1025, 24-29.	2.5	5
53	Spin-dependent and Coriolis interactions by an improved configuration interaction treatment: predissociation of excited fine structure levels of OH/OD. Molecular Physics, 2000, 98, 1713-1727.	1.7	5
54	Theoretical Study of the A2Î£+-X2Î Transition of CCO-. Collection of Czechoslovak Chemical Communications, 2001, 66, 983-990.	1.0	4

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55	Ab initiostudy of the C2O+cation. Molecular Physics, 2007, 105, 1105-1114.	1.7	4
56	Theoretical study of the predissociation of the A2Î state of ZnF including quasi-diabatisation of the spin-orbit coupling. Journal of Chemical Physics, 2012, 137, 164318.	3.0	4
57	Ab initio ro-vibronic spectroscopy of SiCCl ($ilde{X}^2Pi$XÌƒ2Î). Journal of Chemical Physics, 2014, 141, 034305.	3.0	4
58	Multiscale Study of Gas Slip Flows in Nanochannels. Journal of Heat Transfer, 2015, 137, .	2.1	4
59	A theoretical study of the Rennerâ€“Teller effect in the XÌƒ2Îg state of C3â^'. Chemical Physics Letters, 2001, 335, 97-104.	2.6	3
60	Ab initio Study of HZnF. Journal of Physical Chemistry A, 2009, 113, 14615-14624.	2.5	3
61	Spectroscopic properties of trichlorofluoromethane CCl3F calculated by density functional theory. Physical Chemistry Chemical Physics, 2007, 9, 5027.	2.8	2
62	Simulation of the Ãƒ²Î£⁺â€“XÌƒ²Î absorption and emission spectra of the SiCCl radical. Molecular Physics, 2015, 113, 1695-1703.	1.7	2
63	Ab initio investigations on the CaO2+ dication. Computational and Theoretical Chemistry, 2015, 1052, 1-5.	2.5	2
64	Strain-induced friction anisotropy between graphene and molecular liquids. Journal of Chemical Physics, 2017, 146, 014707.	3.0	2
65	Oxidation of Silver Cyanide Ag(CN)₂^{â€“} by the OH Radical: From Ab Initio Calculation to Molecular Simulation and to Experiment. Journal of Physical Chemistry A, 2020, 124, 10787-10798.	2.5	2
66	Raw and processed data used in non-covalent functionalization of single walled carbon nanotubes with Co-porphyrin and Co-phthalocyanine and its effect on field-effect transistor characteristics. Data in Brief, 2021, 38, 107366.	1.0	2
67	Electronic states and rovibrational spectroscopy of the HAlF+ and HAlCl+ cations. Computational and Theoretical Chemistry, 2012, 997, 19-24.	2.5	1
68	Different Time Scales in the Dissociation Dynamics of Core-Excited CF4 by Two Internal Clocks. Physical Review Letters, 2017, 119, 203203.	7.8	1
69	Multiscale Study of Gas Slip Flows in Nanochannels. , 2013, , .		1
70	Velocity Slip and Temperature Jump for Gas Flows Past Anisotropic Surfaces: Analytical Derivation and Numerical Simulation. , 2016, , .		0
71	Imidazole functionalized graphene and carbon nanotubes for CO2 detection. Journal of Molecular Structure, 2022, 1259, 132719.	3.6	0