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	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
2	Imidazole functionalized graphene and carbon nanotubes for CO2 detection. Journal of Molecular Structure, 2022, 1259, 132719.	3.6	0
3	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
4	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
5	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
6	Non-parametric wall model and methods of identifying boundary conditions for moments in gas flow equations. Physics of Fluids, 2018, 30, .	4.0	14
7	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
8	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
9	Strain-induced friction anisotropy between graphene and molecular liquids. Journal of Chemical Physics, 2017, 146, 014707.	3.0	2
10	Different Time Scales in the Dissociation Dynamics of Core-Excited CF4 by Two Internal Clocks. Physical Review Letters, 2017, 119, 203203.	7.8	1
11	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
12	Velocity Slip and Temperature Jump for Gas Flows Past Anisotropic Surfaces: Analytical Derivation and Numerical Simulation. , 2016, , .		0
13	Quasi-particle energies and optical excitations of wurtzite BeO and its nanosheet. Journal of Alloys and Compounds, 2016, 682, 254-262.	5.5	63
14	Rovibrational energy levels of the F^{â˜}(H₂O) and F^{â˜}(D₂O) complexes. Physical Chemistry Chemical Physics, 2016, 18, 17678-17690.	2.8	22
15	Boundary conditions for gas flow problems from anisotropic scattering kernels. Journal of Mathematical Physics, 2015, 56, .	1.1	8
16	Multiscale Study of Gas Slip Flows in Nanochannels. Journal of Heat Transfer, 2015, 137, .	2.1	4
17	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
18	Free-path distribution and Knudsen-layer modeling for gaseous flows in the transition regime. Physical Review E, 2015, 91, 023015.	2.1	17

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19	Simulation of the Ãƒ²Î£⁺â€“XÌƒ²Î absorption and emission spectra of the SiCCl radical. Molecular Physics, 2015, 113, 1695-1703.	1.7	2
20	Ab initio investigations on the CaO2+ dication. Computational and Theoretical Chemistry, 2015, 1052, 1-5.	2.5	2
21	Ab initio ro-vibronic spectroscopy of SiCCl ($ilde{X}^2Pi$XÌƒ2Î). Journal of Chemical Physics, 2014, 141, 034305.	3.0	4
22	Rovibrational energies of B2H2() from an explicitly correlated potential energy surface. Computational and Theoretical Chemistry, 2013, 1025, 24-29.	2.5	5
23	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
24	Theoretical Investigations on CaO Ions: Vibronic States and Photoelectron Spectroscopy. Journal of Physical Chemistry A, 2013, 117, 11254-11260.	2.5	10
25	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
26	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
27	Multiscale Study of Gas Slip Flows in Nanochannels. , 2013, , .		1
28	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
29	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
30	Electronic states and rovibrational spectroscopy of the HAlF+ and HAlCl+ cations. Computational and Theoretical Chemistry, 2012, 997, 19-24.	2.5	1
31	Electronic States, Potential Energy Surface, and Theoretical Spectroscopy of Be₂H₂. Journal of Physical Chemistry A, 2012, 116, 9484-9489.	2.5	9
32	CCSD(T)â€F12 investigations on HBNH and its isotopologues. International Journal of Quantum Chemistry, 2012, 112, 2051-2061.	2.0	7
33	Theoretical Study of the Rovibronic States of CaO. Journal of Molecular Spectroscopy, 2012, 271, 1-9.	1.2	14
34	Molecular Dynamics Simulations of Pressure-Driven Flows and Comparison with Acceleration-Driven Flows. Advances in Mechanical Engineering, 2012, 4, 580763.	1.6	11
35	Theoretical spectroscopy of the HNClâ^' anion. Molecular Physics, 2011, 109, 2655-2662.	1.7	5
36	Ab initio study of the low-lying electronic states of the CaO molecule. Chemical Physics, 2011, 386, 50-55.	1.9	17

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37	Mg2H2: New insight on the Mgâ€“Mg bonding and spectroscopic study. Journal of Chemical Physics, 2011, 134, 054314.	3.0	6
38	A slip model for micro/nano gas flows induced by body forces. Microfluidics and Nanofluidics, 2010, 8, 417-422.	2.2	15
39	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
40	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
41	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
42	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
43	Ab initio Study of HZnF. Journal of Physical Chemistry A, 2009, 113, 14615-14624.	2.5	3
44	Radiative transition probabilities in the state of. Journal of Quantitative Spectroscopy and Radiative Transfer, 2008, 109, 535-548.	2.3	9
45	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:mo>(</mml:mo><mml:mrow><mml:mi mathvariant="normal">Î£</mml:mi></mml:mrow><mml:mrow><mml:mo>+</mml:mo></mml:mrow><mml:mo>)</mml:mo></mml:mrow></mml:math> and of the transition <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si241.gif"	2.0	7
46	di. Chemical Physics Letters, 2008, 458, 24-28. 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
47	Ab initiostudy of the low lying electronic states of ZnF and ZnFâ¯. Journal of Chemical Physics, 2008, 129, 044313.	3.0	8
48	Time-dependent wave packet study ontrans-cisisomerization of HONO driven by an external field. Journal of Chemical Physics, 2007, 127, 164315.	3.0	47
49	Ab initiostudy of the C2O+cation. Molecular Physics, 2007, 105, 1105-1114.	1.7	4
50	Spectroscopic properties of trichlorofluoromethane CCl3F calculated by density functional theory. Physical Chemistry Chemical Physics, 2007, 9, 5027.	2.8	2
51	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
52	Ab initiostudy of the spinâ€“orbit coupling between the A and b3Îuelectronic states of Na2. Molecular Physics, 2007, 105, 1095-1104.	1.7	5
53	Calculation and selective population of vibrational levels with the Multiconfiguration Time-Dependent Hartree (MCTDH) algorithm. Chemical Physics, 2006, 329, 179-192.	1.9	215
54	A theoretical spectroscopic study of HeI and HeBr. Physical Chemistry Chemical Physics, 2005, 7, 1694-1699.	2.8	9

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55	Spinâ€“orbit coupling in the X2Î state of NCS. Chemical Physics Letters, 2004, 398, 123-129.	2.6	11
56	The barrier to inversion of ammonia. Chemical Physics Letters, 2003, 370, 360-365.	2.6	43
57	Theoretical determination of the vibrational levels of NH3+with MULTIMODE. Physical Chemistry Chemical Physics, 2002, 4, 4087-4095.	2.8	10
58	Theoretical enthalpies of formation of large compounds using integrated methods. Physical Chemistry Chemical Physics, 2002, 4, 4096-4102.	2.8	11
59	The vibrational levels of ammonia. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 825-838.	3.9	62
60	The selective population of the vibrational levels of thioformaldehyde. Physical Chemistry Chemical Physics, 2001, 3, 508-513.	2.8	20
61	Theoretical determination of the vibrational levels of NH+3and its isotopomers. Molecular Physics, 2001, 99, 1335-1346.	1.7	11
62	Theoretical Study of the A2Î£+-X2Î Transition of CCO-. Collection of Czechoslovak Chemical Communications, 2001, 66, 983-990.	1.0	4
63	Theoretical study of the Aâ€“X transition in C2Bâ¯. Chemical Physics, 2001, 264, 267-273.	1.9	5
64	A theoretical study of the Rennerâ€“Teller effect in the XÌƒ2Îg state of C3â¯. Chemical Physics Letters, 2001, 335, 97-104.	2.6	3
65	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
66	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
67	Selective vibrational excitations in the OX (X=F, Cl, Br, I) molecules. Physical Chemistry Chemical Physics, 2000, 2, 1117-1122.	2.8	15
68	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
69	Potential energy function and vibrational states of N2CO+. Journal of Chemical Physics, 1999, 111, 4948-4955.	3.0	29
70	Bound electronic states X1Î£+, a3Î and A1Î of C2B-. Physical Chemistry Chemical Physics, 1999, 1, 1827-1832.	2.8	11
71	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