Jaime Rubio-MartÃ-nez

List of Publications by Year
in descending order

134 papers	3,058 citations	185998 28 h-index	214527 47 g-index
138 all docs	138 docs citations	138 times ranked	3130 citing authors

#	Article	IF	Citations
1	Origin of the Large N 1s Binding Energy in X-ray Photoelectron Spectra of Calcined Carbonaceous Materials. Journal of the American Chemical Society, 1996, 118, 8071-8076.	6.6	490
2	Effect of electron correlation on the electrostatic potential distribution of molecules. Journal of the American Chemical Society, 1991, 113, 5203-5211.	6.6	76
3	Madelung fields from optimized point charges forab initiocluster model calculations on ionic systems. Journal of Computational Chemistry, 1993, 14, 680-684.	1.5	74
4	Selected versus complete configuration interaction expansions. Journal of Chemical Physics, 1991, 95, 1877-1883.	1.2	70
5	Theoretical analysis of bonding in monomeric and polymeric C5H5M compounds. Organometallics, 1984, 3, 759-764.	1.1	66
6	Origin of the vibrational shift of CO chemisorbed on Pt(111). Physical Review B, 1995, 52, 12372-12379.	1.1	65
7	Origin of magnetic coupling inLa2CuO4. Physical Review B, 1996, 53, 945-951.	1.1	61
8	On the bonding mechanism of CO to Pt(111) and its effect on the vibrational frequency of chemisorbed CO. Surface Science, 1997, 376, 279-296.	0.8	61
9	Treating large intermediate spaces in the CIPSI method through a direct selected CI algorithm. Theoretica Chimica Acta, 1992, 82, 229-238.	0.9	53
10	Molecular structure and vibrational frequencies of AlxOy (x=1,2; yâ©½3) derived from ab initio calculations. Chemical Physics Letters, 1988, 144, 373-377.	1.2	50
11	Ab initiocluster-model study of the on-top chemisorption of F and Cl on Si(111) and Ge(111) surfaces. Physical Review B, 1985, 31, 8068-8075.	1.1	49
12	Assessment of the Sampling Performance of Multiple-Copy Dynamics versus a Unique Trajectory. Journal of Chemical Information and Modeling, 2016, 56, 1950-1962.	2.5	48
13	Approximate natural orbitals and the convergence of a second order multireference manyâ€body perturbation theory (CIPSI) algorithm. Journal of Chemical Physics, 1988, 89, 6376-6384.	1.2	45
14	The Methylerythritol Phosphate (MEP) Pathway for Isoprenoid Biosynthesis as a Target for the Development of New Drugs Against Tuberculosis. Current Medicinal Chemistry, 2011, 18, 1325-1338.	1.2	43
15	Dynamical and nondynamical correlation effects inabinitiochemisorption cluster model calculations. Ground and low lying states of H on Cu(100) and Ag(100). Journal of Chemical Physics, 1988, 88, 260-271.	1.2	42
16	Comparative Evaluation of MMPBSA and XSCORE To Compute Binding Free Energy in XIAPâ'Peptide Complexes. Journal of Chemical Information and Modeling, 2007, 47, 134-142.	2.5	41
17	Doublet instability and the molecular structure of AlO2. Journal of Computational Chemistry, 1988, 9, 836-843.	1.5	39
18	The nature of the chemical bond in simple oxides: A theoretical journey from the ionic model to the ab initio configuration interaction approach. Journal of Chemical Physics, 1993, 99, 389-396.	1.2	39

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19	Ab initioelectronic structure of PtH+, PtH, Pt2, and Pt2H from a oneâ€electron pseudopotential approach. Journal of Chemical Physics, 1996, 104, 8500-8506.	1.2	36
20	Electronic structure of Rh, RhH, and Rh2 as derived from ab initio (configuration interaction) calculations. Journal of Chemical Physics, 1990, 93, 2603-2610.	1.2	35
21	Direct determination of localized Hartreeâ€“Fock orbitals as a step toward N scaling procedures. Journal of Chemical Physics, 1997, 107, 10044-10050.	1.2	35
22	Electronic and geometrical structures of Pt3 and Pt4. An ab initio one-electron proposal. Chemical Physics Letters, 1994, 217, 283-287.	1.2	34
23	Cu as a one-electron atom: Molecular structure and dissociation energy of CuOH. Chemical Physics Letters, 1985, 119, 397-402.	1.2	33
24	Ab initio selfâ€consistent field and configuration interaction study of Cu5O and Ag5O as models for oxygen chemisorption on Cu(100) and Ag(100). Journal of Chemical Physics, 1989, 91, 5466-5475.	1.2	32
25	The analysis of the chemisorption bond from uncorrelated and correlated cluster model wave functions. Journal of Chemical Physics, 1994, 100, 1988-1994.	1.2	32
26	Molecular Determinants of Bim(BH3) Peptide Binding to Pro-Survival Proteins. Journal of Chemical Information and Modeling, 2012, 52, 2107-2118.	2.5	31
27	Cluster model description of the chemisorption bond: effect of the cluster model electronic state. Surface Science, 1994, 304, 335-342.	0.8	30
28	Nature of bonding of alkali metals to Si(111). Physical Review B, 1995, 51, 1581-1592.	1.1	30
29	On the inversion barriers of group 15 tricoordinate hydrides and halides: An ab initio study using analytical gradients. Computational and Theoretical Chemistry, 1988, 164, 351-361.	1.5	28
30	Chemisorption of group-III metals on the Si(111) and Ge(111) surfaces: Anab initiostudy. Physical Review B, 1990, 42, 5212-5220.	1.1	28
31	Bonding geometry and mechanism of NO adsorbed on Cu2O(111): NO activation by Cu+ cations. Journal of Chemical Physics, 1994, 101, 10134-10139.	1.2	28
32	Neutral versus ionic interactions in ab initio chemisorption cluster model calculations: halogens on mercury. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1989, 267, 243-250.	0.3	27
33	Molecular structure of copper(I) hydroxide and copper hydroxide(1-) (Cu(OH)2-). An ab initio study. The Journal of Physical Chemistry, 1984, 88, 5225-5228.	2.9	26
34	Ab initio cluster model approach to the chemisorption on mercury. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1989, 261, 39-50.	0.3	26
35	The effect of dynamical correlation on the valence wavefunction of molecules: Dressed complete active space self-consistent field calculations. Chemical Physics, 1990, 147, 293-307.	0.9	26
36	Bonding of atomic oxygen to Cu(100) and Ag(100) surfaces: a theoretical comparative study. Surface Science, 1993, 297, 57-65.	0.8	26

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37	Cyclin-dependent kinases 4 and 6 control tumor progression and direct glucose oxidation in the pentose cycle. Metabolomics, 2012, 8, 454-464.	1.4	25
38	Nonempirical cluster-model study of the chemisorption of atomic hydrogen on the (111) surface of diamondlike crystals. Physical Review B, 1986, 34, 7203-7208.	1.1	24
39	Reliability of oneâ€electron approaches in chemisorption cluster model studies: Role of coreâ€polarization and coreâ€“valence correlation effects. Journal of Chemical Physics, 1990, 93, 2521-2529.	1.2	24
40	Ab initio study of the ground and lowâ€lying states of FeH. Journal of Chemical Physics, 1990, 92, 2478-2480.	1.2	24
41	On the use of frozen orbitals in molecular orbital cluster calculations: Cl on Si(111). Chemical Physics Letters, 1985, 120, 513-516.	1.2	23
42	Bonding of atomic oxygen to Cu(100) and Ag(100) surfaces: a study of the nature of the interaction. Surface Science, 1994, 307-309, 107-112.	0.8	23
43	Structural Analysis of the Inhibition of Cdk4 and Cdk6 by p16^{INK4a}through Molecular Dynamics Simulations. Journal of Biomolecular Structure and Dynamics, 2002, 20, 347-358.	2.0	23
44	MINDO/3 potential energy surface for hydrogen-graphite system: Active sites and migration. Surface Science, 1985, 149, 621-629.	0.8	22
45	The importance of correlation effects on the bonding of atomic oxygen on Pt(111). Journal of Chemical Physics, 1996, 105, 7192-7199.	1.2	22
46	Rational Design of New Class of BH3-Mimetics As Inhibitors of the Bcl-x_L Protein. Journal of Chemical Information and Modeling, 2011, 51, 1249-1258.	2.5	22
47	Microwaveâ€Assisted Synthesis of Substituted Pyrrolo[2,3â€d]pyrimidines. European Journal of Organic Chemistry, 2014, 2014, 1514-1524.	1.2	22
48	Chemisorption of atomic aluminum on Si(111): Evidence for an adsorbate-induced relaxation based onab initiocluster-model calculations. Physical Review B, 1988, 38, 10700-10710.	1.1	21
49	Ab Initio Study of the Magnetic Coupling in Na6Fe2S6. Journal of Physical Chemistry A, 1997, 101, 1526-1531.	1.1	21
50	Vibrational frequencies of halogens adsorbed on Ag (100) based on ab initio cluster model calculations. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1986, 200, 47-53.	0.3	20
51	Proteinâ€“protein recognition as a first step towards the inhibition of XIAP and Survivin antiâ€apoptotic proteins. Journal of Molecular Recognition, 2008, 21, 190-204.	1.1	20
52	Convergence of a multireference second-order mbpt method (CIPSI) using a zero-order wavefunction derived from an MS SCF calculation. Chemical Physics Letters, 1986, 126, 98-102.	1.2	19
53	Ground and lowâ€lying states of FeH+ as derived from ab initio selfâ€consistent field and configuration interaction calculations. Journal of Chemical Physics, 1989, 90, 6436-6442.	1.2	19
54	Ab initiovalence-bond cluster model for ionic solids: Alkaline-earth oxides. Physical Review B, 1993, 47, 6207-6215.	1.1	19

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55	Size-consistent selected configuration interaction calculations. A few tests of efficiency. Chemical Physics Letters, 1993, 209, 126-134.	1.2	18
56	Molecular structure, vibrational frequencies and ionization potential of tin dihalides. Chemical Physics Letters, 1986, 123, 528-532.	1.2	17
57	The effect of electron correlation in the interaction of atomic hydrogen with Ben clusters 3â‰nâ‰7. Journal of Chemical Physics, 1986, 84, 3311-3316.	1.2	17
58	An analysis of 3d correlation effects in the bonding of atomic oxygen to Cu(100). Journal of Chemical Physics, 1991, 95, 4225-4229.	1.2	17
59	The nature of the bonding of atomic Al to Si(111): is there a specific site-bond relationship?. Surface Science, 1992, 275, 459-472.	0.8	17
60	Ab initio cluster model study of geometry and bonding character of atomic nitrogen chemisorbed on the Cu(100) and Ag(100) surfaces. Surface Science, 1997, 374, 31-43.	0.8	17
61	Mimicking direct proteinâ€“protein and solvent-mediated interactions in the CDP-methylerythritol kinase homodimer: a pharmacophore-directed virtual screening approach. Journal of Molecular Modeling, 2009, 15, 997-1007.	0.8	17
62	Ab initio molecular structure of Xn,H2n, compounds, (X = Si, Ge, Sn; n = 3, 4). Computational and Theoretical Chemistry, 1984, 110, 131-137.	1.5	16
63	Ab initio study of the superoxides of Group 13 metals. The Journal of Physical Chemistry, 1986, 90, 30-33.	2.9	16
64	The ionicity of halogens chemisorbed on mercury revisited. Journal of Electroanalytical Chemistry, 1993, 359, 105-113.	1.9	16
65	Active sites of Pt surfaces from ab initio cluster model molecular electrostatic potential maps. Electrochimica Acta, 1996, 41, 2275-2283.	2.6	16
66	Theoretical evidence for two geometrical isomers of silver oxide (AgO2). Journal of the American Chemical Society, 1986, 108, 7893-7897.	6.6	15
67	Mixed pseudo-potential approach to the on-top chemisorption of atomic hydrogen on the (100) silver surface. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1987, 216, 29-40.	0.3	15
68	The orthogonal valence bond interpretation of ab initio chemisorption cluster model wavefunctions. Chemical Physics, 1993, 177, 61-67.	0.9	15
69	Title is missing!. Journal of Mathematical Chemistry, 1999, 25, 85-92.	0.7	15
70	Molecular dynamics study of peptide segments of the BH3 domain of the proapoptotic proteins Bak, Bax, Bid and Hrk bound to the Bcl-xLand Bcl-2 proteins. Journal of Computer-Aided Molecular Design, 2004, 18, 13-22.	1.3	14
71	Homology modeling of human Transketolase: Description of critical sites useful for drug design and study of the cofactor binding mode. Journal of Molecular Graphics and Modelling, 2009, 27, 723-734.	1.3	14
72	Effect of the solvent on the conformational behavior of the alanine dipeptide deduced from MD simulations. Journal of Molecular Graphics and Modelling, 2017, 78, 118-128.	1.3	14

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73	Substituted tetrahydroisoquinolines: synthesis, characterization, antitumor activity and other biological properties. European Journal of Medicinal Chemistry, 2018, 145, 51-63.	2.6	14
74	Discovery of Diverse Natural Products as Inhibitors of SARS-CoV-2 M^{pro} Protease through Virtual Screening. Journal of Chemical Information and Modeling, 2021, 61, 6094-6106.	2.5	14
75	Basis-Modified hydrogen atoms as embedding atoms inab initio chemisorption cluster model calculations on Si surfaces. Journal of Computational Chemistry, 1993, 14, 1534-1544.	1.5	13
76	Adiabatic and diabatic representations of potential energy curves for the (NaRb)+ system. Chemical Physics Letters, 1996, 261, 583-590.	1.2	13
77	One-pot synthesis of 4-aminated pyrrolo[2,3-d]pyrimidines from alkynylpyrimidines under metal-catalyst-free conditions. Tetrahedron, 2015, 71, 1207-1214.	1.0	13
78	Identification of Potential Small Molecule Binding Pockets in p38Î± MAP Kinase. Journal of Chemical Information and Modeling, 2017, 57, 2566-2574.	2.5	13
79	An efficient improvement of the string-based direct selected CI algorithm. Theoretica Chimica Acta, 1995, 92, 305-313.	0.9	12
80	Molecular Determinants for the Activation/Inhibition of Bak Protein by BH3 Peptides. Journal of Chemical Information and Modeling, 2020, 60, 1632-1643.	2.5	12
81	On the potential energy surface for collinear OH+2 (4Î£â¯). Journal of Chemical Physics, 1991, 94, 3774-3777.	1.2	11
82	Evidence for two different bonding mechanisms of Al on Si(111). Physical Review B, 1993, 47, 2417-2419.	1.1	11
83	Calculation of proton affinities and absolute gas basicities of X3 group VI triatomics: a density functional study. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 2681.	1.7	11
84	Conformationally Restricted Hydantoinâ€Based Peptidomimetics as Inhibitors of Caspaseâ€3 with Basic Groups Allowed at the S₃ Enzyme Subsite. ChemMedChem, 2008, 3, 979-985.	1.6	11
85	RED: A Set of Molecular Descriptors Based on RÃ©nyi Entropy. Journal of Chemical Information and Modeling, 2009, 49, 2457-2468.	2.5	11
86	Molecular Topology Applied to the Discovery of 1-Benzyl-2-(3-fluorophenyl)-4-hydroxy-3-(3-phenylpropanoyl)-2H-pyrrole-5-one as a Non-Ligand-Binding-Pocket Antiandrogen. Journal of Chemical Information and Modeling, 2014, 54, 2953-2966.	2.5	11
87	Effect of set up protocols on the accuracy of alchemical free energy calculation over a set of ACK1 inhibitors. PLoS ONE, 2019, 14, e0213217.	1.1	11
88	An ab initio study of the interaction of atomic hydrogen with cluster models simulating the (100) and (110) silver surfaces. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1985, 196, 387-395.	0.3	10
89	The cluster model configuration interaction approach to the study of chemisorption on metal and semiconductor surfaces. Computational and Theoretical Chemistry, 1993, 287, 167-178.	1.5	10
90	Synthesis and evaluation of diverse analogs of amygdalin as potential peptidomimetics of peptide T. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 1493-1496.	1.0	10

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91	Differential correlation effects in chemisorption cluster model calculations: an FCI study. Chemical Physics Letters, 1991, 180, 578-582.	1.2	9
92	Diphenyl Urea Derivatives as Inhibitors of Transketolase: A Structure-Based Virtual Screening. PLoS ONE, 2012, 7, e32276.	1.1	9
93	Molecular dynamics analysis of the interaction between the human BCL6 BTB domain and its SMRT, NcoR and BCOR corepressors: The quest for a consensus dynamic pharmacophore. Journal of Molecular Graphics and Modelling, 2014, 50, 142-151.	1.3	9
94	Atomic Level Rendering of DNA-Drug Encounter. Biophysical Journal, 2014, 106, 421-429.	0.2	9
95	Modeling and subtleties of K-Ras and Calmodulin interaction. PLoS Computational Biology, 2018, 14, e1006552.	1.5	9
96	Taking into account non-dynamical correlation effects in ab initio chemisorption cluster model calculations. Computational and Theoretical Chemistry, 1989, 202, 315-324.	1.5	8
97	A numerical test on the size consistency of some multireference configuration interaction approaches. Chemical Physics Letters, 1992, 200, 559-566.	1.2	8
98	The full-CI energy of the NH3 molecule in a DZP basis set. Chemical Physics Letters, 1994, 218, 283-286.	1.2	8
99	Binding of the anticancer drug BI-2536 to human serum albumin. A spectroscopic and theoretical study. Journal of Photochemistry and Photobiology B: Biology, 2017, 172, 77-87.	1.7	8
100	The role of d electrons in ab initio chemisorption cluster model calculations. Atomic hydrogen on Cu(100) and Ag(100). Solid State Communications, 1988, 65, 605-608.	0.9	7
101	Ab initio cluster model approach to the chemisorption of hydrogen on mercury. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1988, 241, 105-112.	0.3	7
102	Quasi-classical trajectory study of the dynamics of the reaction O(3P)+CS2(X1âˆ+g)â†'CS(X1âˆ+)+SO(X3âˆâˆ') using two model potential energy surfaces. Chemical Physics, 1992, 161, 99-126.	0.9	7
103	Reducing CDK4/6-p16INK4a interface. Computational alanine scanning of a peptide bound to CDK6 protein. Proteins: Structure, Function and Bioinformatics, 2006, 63, 797-810.	1.5	7
104	Homology modeling of Mycobacterium tuberculosis 2C-methyl-d-erythritol-4-phosphate cytidylyltransferase, the third enzyme in the MEP pathway for isoprenoid biosynthesis. Journal of Molecular Modeling, 2010, 16, 1061-1073.	0.8	7
105	A theoretical study of relaxation and reconstruction of the (111) surface of diamond. Surface Science, 1985, 162, 169-174.	0.8	6
106	Performance of correlation functionals inab initiochemisorption cluster-model calculations: Alkali metals on Si(111). Physical Review B, 1995, 52, 11998-12005.	1.1	6
107	Predicting binding energies of CDK6 inhibitors in the hit-to-lead process. Theoretical Chemistry Accounts, 2011, 128, 807-823.	0.5	6
108	Design of novel ligands of CDP-methylerythritol kinase by mimicking direct protein-protein and solvent-mediated interactions. Journal of Molecular Recognition, 2011, 24, 71-80.	1.1	6

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109	Interpretation of the chemisorption bond based in the partitioning energy scheme in the RHF-MINDO/3 method: Adatoms on graphite. Computational and Theoretical Chemistry, 1986, 136, 303-312.	1.5	5
110	On the performance of atomic natural orbital basis sets: A full configuration interaction study. Journal of Chemical Physics, 1990, 93, 4982-4985.	1.2	5
111	Energy partitioning using two-electron average matrices. Chemical Physics Letters, 1994, 222, 51-57.	1.2	5
112	Pseudometrics from three-positive semidefinite similarities. Fuzzy Sets and Systems, 2006, 157, 2347-2355.	1.6	5
113	Structural analysis of the inhibition of APRIL by TACI and BCMA through molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2013, 39, 13-22.	1.3	5
114	Shedding light on the binding mechanism of kinase inhibitors BI-2536, Volasetib and Ro-3280 with their pharmacological target PLK1. Journal of Photochemistry and Photobiology B: Biology, 2022, 232, 112477.	1.7	5
115	The molecular structure of bicyclo[1.1.0]tetraarsane from ab initio calculations using analytical gradients. Computational and Theoretical Chemistry, 1987, 150, 283-287.	1.5	4
116	Consequences of chemical bonding on the adiabaticity of gas-surface reactions. Computational and Theoretical Chemistry, 1996, 371, 257-267.	1.5	4
117	Assessment of the performance of cluster analysis grouping using pharmacophores as molecular descriptors. Computational and Theoretical Chemistry, 2005, 727, 81-87.	1.5	4
118	Structure-based approach to the design of BakBH3 mimetic peptides with increased helical propensity. Journal of Molecular Modeling, 2013, 19, 4305-4318.	0.8	4
119	Design of an interface peptide as new inhibitor of human glucose-6-phosphate dehydrogenase. Journal of Molecular Graphics and Modelling, 2014, 49, 110-117.	1.3	4
120	Energy levels in the jj coupling scheme. Journal of Chemical Education, 1986, 63, 476.	1.1	3
121	The aluminiumâ€“acetylene interaction: structure, coordination modes, vibrational frequencies and hyperfine coupling constants. The density functional point of view. Computational and Theoretical Chemistry, 1999, 466, 77-84.	1.5	3
122	Exploring potential energy surfaces with gentlest ascent dynamics in combination with the shrinking dimer method and Newtonian dynamics. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	3
123	Fragment dissolved molecular dynamics: a systematic and efficient method to locate binding sites. Physical Chemistry Chemical Physics, 2021, 23, 3123-3134.	1.3	3
124	Analysis of the basis set and correlation effects on the computation of molecular polarizabilities using molecular polarization maps. Theoretical Chemistry Accounts, 2009, 123, 113-118.	0.5	2
125	A benchmark calculation for the fuzzy c-means clustering algorithm: initial memberships. Journal of Mathematical Chemistry, 2012, 50, 2703-2715.	0.7	2
126	A multistep docking and scoring protocol for congeneric series: Implementation on kinase DFG-out type II inhibitors. Future Medicinal Chemistry, 2018, 10, 297-318.	1.1	2

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127	Multigram scale synthesis of polycyclic lactones and evaluation of antitumor and other biological properties. European Journal of Medicinal Chemistry, 2020, 185, 111807.	2.6	2
128	Insight into the Binding of DFG-out Allosteric Inhibitors to B-Raf Kinase Using Molecular Dynamics and Free Energy Calculations. Current Computer-Aided Drug Design, 2015, 11, 124-136.	0.8	2
129	Non-empirical cluster-model study of the relaxation of (111) surfaces of C, Si, Ge. Computational and Theoretical Chemistry, 1990, 204, 325-329.	1.5	1
130	An ab initio study of the collinear reaction of Fe+ (4F) and Fe+ (6D) with H2. Journal of Chemical Physics, 1991, 94, 4352-4355.	1.2	1
131	Toward understanding calmodulin plasticity by molecular dynamics. Future Medicinal Chemistry, 2019, 11, 975-991.	1.1	1
132	On the Use of the Discrete Constant pH Molecular Dynamics to Describe the Conformational Space of Peptides. Polymers, 2021, 13, 99.	2.0	1
133	Reliability of atomic natural orbital basis sets in calculations involving pseudopotentials. Journal of Computational Chemistry, 1992, 13, 148-154.	1.5	0
134	Unravelling Constant pH Molecular Dynamics in Oligopeptides with Explicit Solvation Model. Polymers, 2021, 13, 3311.	2.0	0