

List of publications

90. **Monika Musiał**, Stanisław A. Kucharski, "Multireference Fock Space Coupled Cluster Method for the (3,0) Sector", *J. Phys. Chem. A*, **128**, 9670-9681 (2024).
89. Grzegorz Skrzyński, **Monika Musiał**, "Fock Space Coupled-Cluster Method for the Ground and Excited States of the NaMg⁺ Molecular Cation", *J. Phys. Chem. A*, **128**, 6972-6980 (2024).
88. Grzegorz Skrzyński, **Monika Musiał**, "An Intruder-free Fock Space Coupled-Cluster Study of the Potential Energy Curves of LiMg⁺ within the (2,0) sector", *Molecules*, **29**, 2364-1-17 (2024).
87. Grzegorz Skrzyński, **Monika Musiał**, "Benchmark study of the electronic states of LiRb molecule: ab initio calculations with the Fock space coupled cluster approach", *Molecules*, **28**, 7645-1-20 (2023).
86. Grzegorz Skrzyński, **Monika Musiał**, "Potential energy curves of the LiRb⁺ molecular ion from ab initio calculations with all electrons correlated", *Adv. Quantum Chem.*, **88**, 213-227 (2023).
85. **Monika Musiał**, Stanisław A. Kucharski, "Advanced models of coupled cluster theory for the ground, excited and ionized states", *Adv. Quantum Chem.: Polish Quantum Chemistry from Kołos to now*, **87**, 73-113 (2023).
84. **Monika Musiał**, Anna Bewicz, Stanisław A. Kucharski, "Potential energy curves for electronic states of the sodium dimer with multi-reference coupled cluster calculations", *Mol. Phys.*, DOI:10.1080/00268976.2022.2106320 (2022).
83. Magdalena Tomanek, **Monika Musiał**, Stanisław A. Kucharski, "Fock-space coupled cluster method for potential energy curves of KH and its cation", *Adv. Quantum Chem.*, **83**, 135-138 (2021).

82. Denis Bokhan, Alexander S. Bednyakov, **Monika Musiał**, Ajith Perera, Dmitrii N. Trubnikov, "Explicitly correlated Fock-space coupled-cluster singles and doubles method for (1,1), (0,2), and (2,0) sectors", *J. Chem. Phys.*, **155**, 014107–1-14 (2021).
81. **Monika Musiał**, Stanisław A. Kucharski, Anna Bewicz, Patrycja Skupin, Magdalena Tomanek, "Electronic states of NaLi molecule: Benchmark results with Fock space coupled cluster approach", *J. Chem. Phys.*, **154**, 054109–1-14 (2021).
80. **Monika Musiał**,
Quantum Chemistry and Dynamics of Excited States: Methods and Applications, "Equation-of-Motion Coupled-Cluster Models", p. 77-108, Leticia Gonzalez and Roland Lindh. (eds.), John Wiley and Sons Ltd (2020).
79. Michał Lesiuk, **Monika Musiał**, Robert Moszynski, "Potential-energy curve for the $a^3\Sigma_u^+$ state of a lithium dimer with Slater-type orbitals", *Phys. Rev. A*, **102**, 062806–1-11 (2020).
78. Leszek Meissner, **Monika Musiał**, Stanisław A. Kucharski, "Extension of the Fock-space coupled-cluster method with singles and doubles to the three-valence sector", *J. Chem. Phys.*, **153**, 114115–1-12 (2020).
77. **Monika Musiał**, Leszek Meissner, Justyna Cembrzyńska, "The intermediate Hamiltonian Fock-space coupled-cluster method with approximate evaluation of the three-body effects", *J. Chem. Phys.*, **151**, 184102–1-17 (2019).
76. M. Lesiuk, M. Przybytek, J. G. Balcerzak **M. Musiał**, R. Moszynski, "Ab initio Potential Energy Curve for the Ground State of Beryllium Dimer", *J. Chem. Theory Comput.*, **15**, 2470-2480 (2019).
75. A. Lisoń, **M. Musiał**, S. A. Kucharski, "Potential energy curves of the NaH molecule and its cation with the Fock space coupled cluster method", *Adv. Quantum Chem.*, **79**, 221-237 (2019).

74. M. Musiał, A. Bewicz, P. Skupin, S. A. Kucharski, "Potential energy curves for the LiK^+ and NaK^+ molecular ions with the coupled cluster method", *Adv. Quantum Chem.*, **76**, 333-349 (2018).
73. A. Bewicz, M. Musiał, S. A. Kucharski, "Potential energy curves of the Na_2^+ molecular ion from all electron ab initio relativistic calculations", *Mol. Phys.*, **115**, 2649-2657 (2017).
72. P. Skupin, M. Musiał, S. A. Kucharski, "Potential energy curves for the Low-Lying Electronic States of K_2^+ from ab initio Calculations with All Electrons Correlated", *J. Phys. Chem. A*, **121**, 1480-1486 (2017).
71. M. Musiał, Ł. Lupa, S. A. Kucharski, "Fock space coupled cluster study of the $1^1\Pi_g$ state of the Li_2 molecule", *Mol. Phys.*, **115**, 579-586 (2017).
70. M. Musiał, Ł. Lupa, S. A. Kucharski, "Equation-of-motion coupled cluster method for the description of the high spin excited states", *J. Chem. Phys.*, **144**, 154105-1-9 (2016).
69. M. Musiał, P. Skupin, A. Motyl, "Potential energy curves of NaK molecule from all-electron multireference coupled cluster calculations", *Adv. Quantum Chem.*, **73**, 250-262 (2016).
68. M. Musiał, A. Motyl, P. Skupin, S. A. Kucharski, "Potential energy curves for the low lying electronic states of KLi with Fock space coupled cluster method", *Adv. Quantum Chem.*, **72**, 201-216 (2016).
67. T. Grining, M. Tomza, M. Lesiuk, M. Przybytek, M. Musiał, R. Moszynski, M. Lewenstein, P. Massignan, "Crossover between few and many fermions in a harmonic trap", *Phys. Rev. A*, **92**, 061601 (2015).
66. T. Grining, M. Tomza, M. Lesiuk, M. Przybytek, M. Musiał, P. Massignan, M. Lewenstein, R. Moszynski, "Many interacting fermions in a one-dimensional harmonic trap: a quantum-chemical treatment", *New J. Phys.*, **17**, 115001 (2015).

65. M. Musiał, M. Medrek, S. A. Kucharski, "Potential energy curves of Li_2^+ from all electron EA-EOM-CCSD calculations", *Mol. Phys.*, **113**, 2943 (2015).
64. M. Lesiuk, M. Przybytek, M. Musiał, B. Jeziorski, R. Moszynski, "Calculation of two-centre, two-electron integrals over Slater-type orbitals revised. III. Case study of the beryllium dimer", *Phys. Rev. A*, **91**, 012510 (2015).
63. D. Bokhan, M. Musiał, R. J. Bartlett, "Equation-of-motion coupled cluster method for ionized states with partial inclusion of connected assesment of the accuracy in regular and explicitly -correlated approaches", *Chem. Phys. Lett.*, **610**, 173-178 (2014).
62. M. Musiał, S. A. Kucharski, "Double Electron Affinity for Potential Energy Curves of Closed Shell Molecules", *Lecture Notes in Enginnering and Computer Science - WCECS San Francisco 2014*, **1**, 190-195 (2014).
61. M. Musiał, Ł. Lupa, S. A. Kucharski, "Equation-of-motion coupled cluster double electron attachment method for high spin calculations", *J. Chem. Phys.*, **140**, 114107-1-7 (2014).
60. M. Musiał, S. A. Kucharski, "First principle calculations of the potential energy curves for electronic states of the lithium dimer", *J. Chem. Theory Comput.*, **10**, 1200-1211 (2014).
59. P. Mieszczanin, M. Musiał, S. A. Kucharski, "Potential energy curves via double electron affinity calculations: example of NaLi molecule", *Mol. Phys.*, **112**, 726 (2014).
58. M. Olszówka, M. Musiał, "Coupled cluster calculations in the (0,2) and (2,0) sectors of the Fock space for the lowest electronic states of the O_2 molecule", *Mol. Phys.*, **112**, 609 (2014).
57. M. Musiał, J. Cembrzyńska, L. Meissner, "Potential energy curves via double ionization potential calculations: example of HF molecule", *Adv. Quantum Chem.*, **68**, 153-172 (2014).

56. I. Mikhaylov, **M. Musiał**, A. M. Masunov, "What is the Best Way to Extract Permanent Dipole Moments and Energies of Excited States from Density Functional Theory? Comparison with Coupled Cluster Equation of Motion in Case of para-Nitroaniline", *Comput. Theoret. Chem.*, **1019**, 23-32 (2013).
55. **M. Musiał**, K. Kowalska-Szojda, D. Lyakh, R. J. Bartlett, "Potential energy curves via double electron affinity calculations: dissociation of alkali metal dimers", *J. Chem. Phys.*, **138**, 194103-1-8 (2013).
54. M. Tomza, W. Skomorowski, **M. Musiał**, R. González-Férez, Ch. P. Koch, R. Moszynski, "Interatomic potentials, electronic properties, and spectroscopy of the ground and excited states of the Rb₂ molecule: Ab initio calculations and effects of a non-resonant field", *Mol. Phys.*, **111**, 1781-1797 (2013).
53. **M. Musiał**, M. Olszówka, D. I. Lyakh, R. J. Bartlett, "The equation-of-motion coupled cluster method for triple electron attached states", *J. Chem. Phys.*, **137**, 174102-1-9 (2012).
52. M. Tomza, M. H. Goerz, **M. Musiał**, R. Moszynski, Ch. P. Koch, "Optimized production of ultracold ground-state molecules: Stabilization employing potentials with ion-pair character and strong spin-orbit coupling", *Phys. Rev. A*, **86**, 043424 (2012).
51. **M. Musiał**, Ł. Lupa, K. Szopa, S. A. Kucharski, "Potential energy curves via double ionization potential calculations: example of 1,2-diazene molecule", *Struct. Chem.*, **23**, 1377-1382 (2012).
50. **M. Musiał**, "Multi-reference Fock space coupled-cluster method in standard and an intermediate Hamiltonian formulation for the (2,0) sector", *J. Chem. Phys.*, **136**, 134111 (2012).
49. D. Lyakh, **M. Musiał**, V. Lotrich, R. J. Bartlett, "Multireference nature of chemistry: the coupled-cluster view", *Chem. Rev.*, **112**, 182 (2012).

48. M. Musiał, S. A. Kucharski, R. J. Bartlett, "Multi-reference double electron attached coupled cluster method with full inclusion of the connected triple excitations: MR-DA-CCSDT", *J. Chem. Theory Comput.*, **7**, 3088-3096 (2011).
47. M. Musiał, R. J. Bartlett, "Multi-reference Fock space coupled-cluster method in the intermediate Hamiltonian formulation for potential energy surfaces", *J. Chem. Phys.*, **135**; 044121-1-8 (2011) and in *Virtual Journal of Biological Physics Research*, **22**, August 1 (2011).
46. M. Musiał, A. Perera, R. J. Bartlett, "Multireference coupled-cluster theory: the easy way", *J. Chem. Phys.*, **134**, 114108-1-10 (2011).
45. M. Musiał, R. J. Bartlett, "Charge-transfer separability and size-extensivity in the equation-of-motion coupled cluster method: EOM-CCx", *J. Chem. Phys.*, **134**, 034106-1-12 (2011).
44. L. Meissner, M. Musiał, *Recent Progress in Coupled Cluster Methods*, "Intermediate Hamiltonian Formulations of the Fock-Space Coupled-Cluster Method: Details, Comparisons, Examples", p. 395-428, P. Carsky et al. (eds.), Springer (2010).
43. R. J. Bartlett, M. Musiał, V. Lotrich, T. Kuś, *Recent Progress in Coupled Cluster Methods*, "The Yearn to be Hermitian", p. 1-36, P. Carsky et al. (eds.), Springer (2010).
42. S. A. Kucharski, M. Musiał, "Connected quadruple excitations in the coupled-cluster theory", *Mol. Phys.*, **108**, 2975-2985 (2010).
41. M. Musiał, "The excited, ionized and electron attached states within the EOM-CC approach with full inclusion of connected triple excitations", *Mol. Phys.*, **108**, 2921-2931 (2010).

40. M. Musiał, R. J. Bartlett, "Improving upon CCSD(TQ_f) for potential energy surfaces: ACCSD(TQ_f) models", *J. Chem. Phys.*, **133**, 104102-1-7 (2010).
39. M. Jaworska, M. Musiał, T. Pluta, *Wybrane zagadnienia Chemii kwantowej*, "Metody obliczeniowe chemii kwantowej uwzględniające korelację elektronową", MM: 85-206, Uniwersytet Śląski, Katowice (2009).
38. M. Musiał, S. A. Kucharski, P. Zerzucha, T. Kuś, R. J. Bartlett, "Excited and ionized states of the ozone molecule with full triples coupled cluster methods", *J. Chem. Phys.*, **131**, 194101-1-10 (2009).
37. M. Musiał, "Efficient realization of the Fock-space coupled-cluster method with connected triple excitations", *Chem. Phys. Lett.*, **470**, 358-362 (2009).
36. M. Musiał, R. J. Bartlett, "Spin-free Intermediate Hamiltonian Fock-space coupled-cluster theory with full inclusion of triple excitations for RHF based triplet states", *J. Chem. Phys.*, **129**, 244111-1-6 (2008).
35. M. Musiał, R. J. Bartlett, "Multireference Fock-space coupled-cluster and Equation-of-Motion coupled-cluster theories: the detailed interconnections", *J. Chem. Phys.*, **129**, 134105-1-12 (2008).
34. M. Musiał, R. J. Bartlett, "Intermediate Hamiltonian Fock-space multireference coupled-cluster method with full triples for calculation of excitation energies", *J. Chem. Phys.*, **129**, 044101-1-10 (2008).
33. M. Musiał, R. J. Bartlett, "Benchmark calculations of the Fock-space coupled cluster single, double, and triple excitation method in the intermediate Hamiltonian formulation for electronic excitation energies", *Chem. Phys. Lett.*, **457**, 267-270 (2008).
32. K. Szopa, M. Musiał, S. A. Kucharski, "Coupled cluster study of the energetics and properties of diazene isomers", *Int. J. Quantum Chem.*, **108**, 2108 (2008).

31. M. Musiał, "EOM-CCSDT study of the low-lying ionization potentials of CO₂, CS₂ and OCS",
AIP conference proceedings, **963 Vol.2 Part A**, 98-101 (2007).
30. M. Musiał, R. J. Bartlett, "Addition by Subtraction in Coupled Cluster Theory II. Equation-of-motion coupled cluster method for excited, ionized and electron-attached states based on nCC ground state wave function",
J. Chem. Phys., **127**, 024106-1-9 (2007).
29. R. J. Bartlett, M. Musiał, "Coupled-Cluster theory in Quantum Chemistry",
Rev. Mod. Phys., **79**, 291-352 (2007).
28. R. J. Bartlett, M. Musiał, "Addition by subtraction in coupled-cluster theory: A reconsideration of the CC and CI interface and the nCC hierarchy",
J. Chem. Phys., **125**, 204105-1-17 (2006).
27. M. Musiał, K. Kowalska, R. J. Bartlett, "Accurate calculation of vibrational frequencies in the excited states with full EOM-CCSDT method",
J. Mol. Struct. (THEOCHEM), **768**, 103-109 (2006).
26. S. Coussan, Y. Ferro, A. Trivella, P. Roubin, R. Wieczorek, C. Manca, P. Piecuch, K. Kowalski, M. Włoch, S. A. Kucharski, M. Musiał, "Experimental and theoretical UV characterization of acetylacetone and its isomers",
J. Phys. Chem. A, **110**, 3920-3926 (2006).
25. K. Kowalska, M. Musiał, S. A. Kucharski, "Harmonic and anharmonic frequencies in the excited states with the equation-of-motion coupled cluster method",
Annals of the Polish Chemical Society, **1**, 578-581 (2005).
24. M. Musiał, L. Meissner, "The Fock-space coupled-cluster method in the calculation of excited state properties",
Collect. Czech. Chem. Commun., **70**, 811-825 (2005).
23. M. Musiał, R. J. Bartlett, "A critical comparison of various connected quadruple excitation approximations in the coupled-cluster treatment

- of bond breaking”,
J. Chem. Phys., **122**, 224102-1-9 (2005) and in
Virtual Journal of Biological Physics Research, **9**, June 15 (2005).
22. M. Musiał, L. Meissner, S. A. Kucharski, R. J. Bartlett, ”Molecular applications of intermediate Hamiltonian Fock-space coupled-cluster method for calculation of excitation energies”,
J. Chem. Phys., **122**, 224110-1-10 (2005).
21. M. Musiał, ”Electronic structure of CN^- using Equation-Of-Motion Coupled Cluster method”,
Mol. Phys., **103**, 2055-2060 (2005).
20. R. M. Olson, S. Varganov, M. S. Gordon, H. Metiu, S. Chretien, P. Piecuch, K. Kowalski, S. A. Kucharski, M. Musiał, ”Where Does the Planar-to-Nonplanar Turnover Occur in Small Gold Clusters?”,
J. Amer. Chem. Soc., **127**, 1049-1052 (2005).
19. P. Piecuch, K. Kowalski, I. S. O. Pimienta, P. D. Fan, M. Lodriguito, M. J. McGuire, S. A. Kucharski, T. Kuś, M. Musiał, ”Method of moments of coupled-cluster equations: A new formalism for designing accurate electronic structure methods for ground and excited states”,
Theor. Chem. Acc., **112**, 349-393 (2004).
18. M. J. McGuire, P. Piecuch, K. Kowalski, S. A. Kucharski, M. Musiał, ”Renormalized Coupled-Cluster Calculations of Reactive Potential Energy Surfaces: The BeFH System”,
J. Phys. Chem. A., **108**, 8878-8893 (2004).
17. M. Musiał, S. A. Kucharski, ”Connected triple excitations in the calculation of the adiabatic excitation energies in the equation-of-motion coupled cluster theory”,
Struct. Chem., **15**, 421-426 (2004).
16. M. Musiał, R. J. Bartlett, ”Fock space multireference coupled cluster method with full inclusion of connected triples for excitation energies”,
J. Chem. Phys., **121**, 1670-1675 (2004).
15. M. Musiał, S. A. Kucharski, R. J. Bartlett, ”Approximate inclusion of the T_3 and R_3 operators in the equation-of-motion coupled cluster

- method”,
Adv. Quantum Chem., **47**, 209-222 (2004).
14. R. L. DeKock, M. J. McGuire, P. Piecuch, W. D. Allen, H. F. Schaefer III, K. Kowalski, S. A. Kucharski, **M. Musiał**, A. R. Bonner, S. A. Spronk, D. B. Lawson, S. L. Laursen, “The Electronic Structure and Vibrational Spectrum of *trans*-HNOO”,
J. Phys. Chem. A., **108**, 2893-2903 (2004).
 13. **M. Musiał**, R. J. Bartlett, “EOM-CCSDT study of the low-lying ionization potentials of ethylene, acetylene and formaldehyde”,
Chem. Phys. Lett., **384**, 210-214 (2004).
 12. M. Włoch, **M. Musiał**, S. A. Kucharski, “Connected triple excitations in the Equation-of-Motion Coupled Cluster calculations of the energies and properties of excited states: HCN molecule”,
Comp. Met. Sci. Techn., **9**, 163-172 (2003).
 11. M. Tobita, S. A. Perera, **M. Musiał**, R. J. Bartlett, M. Nooijen, J. S. Lee, “A critical comparison of single- and multi-reference coupled-cluster methods. Geometry, harmonic frequencies, and excitation energies of N₂O₂”,
J. Chem. Phys., **119**, 10713-10723 (2003).
 10. **M. Musiał**, R. J. Bartlett, “Equation-of-motion coupled cluster method with full inclusion of the connected triple excitations for electron attached states: EA-EOM-CCSDT”,
J. Chem. Phys., **119**, 1901-1908 (2003).
 9. **M. Musiał**, S. A. Kucharski, R. J. Bartlett, “Equation-of-motion coupled cluster method with full inclusion of the connected triple excitations for ionized states: IP-EOM-CCSDT”,
J. Chem. Phys., **118**, 1128-1136 (2003).
 8. P. Piecuch, S. A. Kucharski, K. Kowalski, **M. Musiał**, “Efficient computer implementation of the renormalized coupled cluster methods. The R-CCSD[T], R-CCSD(T), CR-CCSD[T] and CR-CCSD(T) approaches”,
Comp. Phys. Com., **149**, 71-96 (2002).

7. M. Musiał, S. A. Kucharski, R. J. Bartlett, "Formulation and Implementation of the Full Coupled-Cluster Method through Pentuple Excitations", *J. Chem. Phys.*, **116**, 4382-4388 (2002).
6. M. Musiał, S. A. Kucharski i R. J. Bartlett, "Diagrammatic structure of the general coupled cluster equations", *Mol. Phys.*, **100**, 1867-1872 (2002).
5. M. Włoch, M. Musiał, S. A. Kucharski, "Equation-of-Motion Coupled-Cluster method with full inclusion of the triple excitations", *Annals of the Polish Chemical Society*, **1**, 255 (2001).
4. S. A. Kucharski, M. Musiał, "High accuracy correlation corrections for the molecular energies and properties with the coupled cluster method", *Annals of the Polish Chemical Society*, **1**, 290 (2001).
3. S. A. Kucharski, M. Włoch, M. Musiał, R. J. Bartlett, "Coupled-cluster theory for excited electronic states: the full equation-of-motion coupled cluster single, double, and triple excitation method", *J. Chem. Phys.*, **115**, 8263-8266 (2001).
2. M. Musiał, S. A. Kucharski, R. J. Bartlett, "Coupled cluster study of the triple bond", *J. Mol. Struct. (THEOCHEM)*, **547**, 269-278 (2001).
1. M. Musiał, S. A. Kucharski, R. J. Bartlett, " T_5 operator in coupled cluster calculations", *Chem. Phys. Lett.*, **320**, 542-548 (2000).