

Full Publication List of Sergiy Bubin

- [1] S. Bubin and L. Adamowicz, “Variational calculations of excited states with zero total angular momentum (vibrational spectrum) of H_2 without use of the Born–Oppenheimer approximation,” *J. Chem. Phys.* **118**, 3079 (2003).
- [2] M. Cafiero, S. Bubin, and L. Adamowicz, “Non-Born-Oppenheimer calculations of atoms and molecules,” *Phys. Chem. Chem. Phys.* **5**, 1491 (2003).
- [3] S. Bubin and L. Adamowicz, “Non-Born–Oppenheimer study of positronic molecular systems: $e^+\text{LiH}$,” *J. Chem. Phys.* **120**, 6051 (2004).
- [4] S. Bubin and L. Adamowicz, “Nonrelativistic molecular quantum mechanics without approximations: Electron affinities of LiH and LiD ,” *J. Chem. Phys.* **121**, 6249 (2004).
- [5] S. Bubin, M. Cafiero, and L. Adamowicz, “Quantum mechanical calculations on molecules containing positrons,” in *Fundamental World of Quantum Chemistry*, Vol. 3, edited by E. J. Brändas and E. S. Kryachko (Kluwer, 2004) p. 521.
- [6] S. Bubin, E. Bednarz, and L. Adamowicz, “Charge asymmetry in HD^+ ,” *J. Chem. Phys.* **122**, 041102 (2005).
- [7] S. Bubin and L. Adamowicz, “Nucleus-nucleus correlation function in non-Born-Oppenheimer molecular calculations: vibrationally excited states of HD^+ ,” *Chem. Phys. Lett.* **403**, 185 (2005).
- [8] E. Bednarz, S. Bubin, and L. Adamowicz, “Integrals for non-Born–Oppenheimer calculations of molecules with three nuclei,” *Mol. Phys.* **103**, 1169 (2005).
- [9] E. Bednarz, S. Bubin, and L. Adamowicz, “Non-Born–Oppenheimer variational calculations of HT^+ bound states with zero angular momentum,” *J. Chem. Phys.* **122**, 164302 (2005).
- [10] S. Bubin, M. Cafiero, and L. Adamowicz, “Non-Born-Oppenheimer variational calculations of atoms and molecules with explicitly correlated Gaussian basis functions,” *Adv. Chem. Phys.* **131**, 377 (2005).
- [11] M. Pavanello, S. Bubin, M. Molski, and L. Adamowicz, “Non-Born–Oppenheimer calculations of the pure vibrational spectrum of HeH^+ ,” *J. Chem. Phys.* **123**, 104306 (2005).
- [12] S. Bubin, L. Adamowicz, and M. Molski, “An accurate non-Born–Oppenheimer calculation of the first purely vibrational transition in LiH molecule,” *J. Chem. Phys.* **123**, 134310 (2005).
- [13] S. Bubin and L. Adamowicz, “Matrix elements of N -particle explicitly correlated Gaussian basis functions with complex exponential parameters,” *J. Chem. Phys.* **124**, 224317 (2006).
- [14] M. Stanke, D. Kędziera, M. Molski, S. Bubin, M. Barysz, and L. Adamowicz, “Convergence of Experiment and Theory on the Pure Vibrational Spectrum of HeH^+ ,” *Phys. Rev. Lett.* **96**, 233002 (2006).
- [15] D. Kędziera, M. Stanke, S. Bubin, M. Barysz, and L. Adamowicz, “Darwin and mass-velocity relativistic corrections in non-Born-Oppenheimer variational calculations,” *J. Chem. Phys.* **125**, 084303 (2006).

- [16] D. Kędziera, M. Stanke, S. Bubin, M. Barysz, and L. Adamowicz, “Darwin and mass-velocity relativistic corrections in the non-Born-Oppenheimer calculations of pure vibrational states of H_2 ,” *J. Chem. Phys.* **125**, 014318 (2006).
- [17] S. Bubin and L. Adamowicz, “Non-Born-Oppenheimer variational calculation of the ground-state vibrational spectrum of LiH^+ ,” *J. Chem. Phys.* **125**, 064309 (2006).
- [18] S. Bubin and L. Adamowicz, “Nonrelativistic variational calculations of the positronium molecule and the positronium hydride,” *Phys. Rev. A* **74**, 052502 (2006).
- [19] M. Stanke, D. Kędziera, S. Bubin, and L. Adamowicz, “Relativistic corrections to the non-Born-Oppenheimer energies of the lowest singlet Rydberg states of ^3He and ^4He ,” *J. Chem. Phys.* **126**, 194312 (2007).
- [20] S. Bubin, M. Stanke, D. Kędziera, and L. Adamowicz, “Relativistic corrections to the ground-state energy of the positronium molecule,” *Phys. Rev. A* **75**, 062504 (2007).
- [21] S. Bubin and L. Adamowicz, “Calculations of the ground states of BeH and BeH^+ without the Born-Oppenheimer approximation,” *J. Chem. Phys.* **126**, 214305 (2007).
- [22] M. Stanke, D. Kędziera, S. Bubin, and L. Adamowicz, “Ionization potential of ^9Be calculated including nuclear motion and relativistic corrections,” *Phys. Rev. A* **75**, 052510 (2007).
- [23] M. Stanke, D. Kędziera, S. Bubin, and L. Adamowicz, “Lowest Excitation Energy of ^9Be ,” *Phys. Rev. Lett.* **99**, 043001 (2007).
- [24] S. Bubin, M. Stanke, D. Kędziera, and L. Adamowicz, “Improved calculations of the lowest vibrational transitions in HeH^+ ,” *Phys. Rev. A* **76**, 022512 (2007).
- [25] M. Stanke, D. Kędziera, S. Bubin, and L. Adamowicz, “Electron affinity of ^7Li calculated with the inclusion of nuclear motion and relativistic corrections,” *J. Chem. Phys.* **127**, 134107 (2007).
- [26] M. Stanke, D. Kędziera, S. Bubin, M. Molski, and L. Adamowicz, “Lowest vibrational states of $^4\text{He}^3\text{He}^+$: Non-Born-Oppenheimer calculations,” *Phys. Rev. A* **76**, 052506 (2007).
- [27] M. Pavanello, M. Cafiero, S. Bubin, and L. Adamowicz, “Accurate Born–Oppenheimer calculations of the low-lying $c^3\Sigma_g^+$ and $a^3\Sigma_u^+$ excited states of helium dimer,” *Int. J. Quantum Chem.* **108**, 2291 (2008).
- [28] M. Stanke, D. Kędziera, S. Bubin, M. Molski, and L. Adamowicz, “Orbit-orbit relativistic corrections to the pure vibrational non-Born-Oppenheimer energies of H_2 ,” *J. Chem. Phys.* **128**, 114313 (2008).
- [29] M. Stanke, D. Kędziera, S. Bubin, and L. Adamowicz, “Complete α^2 relativistic corrections to the pure vibrational non-Born-Oppenheimer energies of HeH^+ ,” *Phys. Rev. A* **77**, 022506 (2008).
- [30] S. Bubin and L. Adamowicz, “Energy and energy gradient matrix elements with N -particle explicitly correlated complex Gaussian basis functions with $L = 1$,” *J. Chem. Phys.* **128**, 114107 (2008).
- [31] M. Stanke, J. Komasa, D. Kędziera, S. Bubin, and L. Adamowicz, “Three lowest S states of $^9\text{Be}^+$ calculated with including nuclear motion and relativistic and QED corrections,” *Phys. Rev. A* **77**, 062509 (2008).
- [32] M. Stanke, J. Komasa, D. Kędziera, S. Bubin, and L. Adamowicz, “Accuracy limits on the description of the lowest S excitation in the Li atom using explicitly correlated Gaussian basis functions,” *Phys. Rev. A* **78**, 052507 (2008).

- [33] S. Bubin and L. Adamowicz, “Calculations of low-lying 1P states of the beryllium atom,” *Phys. Rev. A* **79**, 022501 (2009).
- [34] M. Stanke, S. Bubin, M. Molski, and L. Adamowicz, “Non-Born-Oppenheimer calculations of the lowest vibrational energy of HD including relativistic corrections,” *Phys. Rev. A* **79**, 032507 (2009).
- [35] S. Bubin, F. Leonarski, M. Stanke, and L. Adamowicz, “Charge asymmetry in pure vibrational states of the HD molecule,” *J. Chem. Phys.* **130**, 124120 (2009).
- [36] M. Stanke, S. Bubin, and L. Adamowicz, “Fundamental vibrational transitions of the $^3\text{He}^4\text{He}^+$ and $^7\text{LiH}^+$ ions calculated without assuming the Born-Oppenheimer approximation and with including leading relativistic corrections,” *Phys. Rev. A* **79**, 060501 (2009).
- [37] S. Bubin, F. Leonarski, M. Stanke, and L. Adamowicz, “Non-adiabatic corrections to the energies of the pure vibrational states of H_2 ,” *Chem. Phys. Lett.* **477**, 12 (2009).
- [38] S. Bubin, M. Stanke, and L. Adamowicz, “Non-Born–Oppenheimer calculations of the BH molecule,” *J. Chem. Phys.* **131**, 044128 (2009).
- [39] M. Stanke, J. Komasa, S. Bubin, and L. Adamowicz, “Five lowest 1S states of the Be atom calculated with a finite-nuclear-mass approach and with relativistic and QED corrections,” *Phys. Rev. A* **80**, 022514 (2009).
- [40] K. L. Sharkey, M. Pavanello, S. Bubin, and L. Adamowicz, “Algorithm for quantum-mechanical finite-nuclear-mass variational calculations of atoms with two p electrons using all-electron explicitly correlated Gaussian basis functions,” *Phys. Rev. A* **80**, 062510 (2009).
- [41] S. Bubin, J. Komasa, M. Stanke, and L. Adamowicz, “Isotope shift in the electron affinity of lithium,” *J. Chem. Phys.* **131**, 234112 (2009).
- [42] S. Bubin, J. Komasa, M. Stanke, and L. Adamowicz, “Isotope shifts of the $1s^22s^2(^1S_0) \rightarrow 1s^22p^2(^1S_0)$ transition in the doubly ionized carbon ion C^{2+} ,” *Phys. Rev. A* **81**, 052504 (2010).
- [43] S. Bubin, J. Komasa, M. Stanke, and L. Adamowicz, “Isotope shifts of the three lowest 1S states of the B^+ ion calculated with a finite-nuclear-mass approach and with relativistic and quantum electrodynamics corrections,” *J. Chem. Phys.* **132**, 114109 (2010).
- [44] K. L. Sharkey, S. Bubin, and L. Adamowicz, “Analytical energy gradient in variational calculations of the two lowest 3P states of the carbon atom with explicitly correlated Gaussian basis functions,” *J. Chem. Phys.* **132**, 184106 (2010).
- [45] S. Bubin, M. Stanke, M. Molski, and L. Adamowicz, “Accurate non-Born-Oppenheimer calculations of the lowest vibrational energies of D_2 and T_2 with including relativistic corrections,” *Chem. Phys. Lett.* **494**, 21 (2010).
- [46] S. Bubin and K. Varga, “Calculation of transmission probability by solving an eigenvalue problem,” *J. Phys. Condens. Matter* **22**, 465306 (2010).
- [47] S. Bubin, M. Stanke, and L. Adamowicz, “Lower vibrational transitions of the $^3\text{He}^4\text{He}^+$ ion calculated without the Born-Oppenheimer approximation and with leading relativistic corrections,” *Chem. Phys. Lett.* **500**, 229 (2010).
- [48] K. L. Sharkey, S. Bubin, and L. Adamowicz, “An algorithm for calculating atomic D states with explicitly correlated Gaussian functions,” *J. Chem. Phys.* **134**, 044120 (2011).

- [49] S. Bubin, M. Stanke, and L. Adamowicz, “Vibrational transitions of the ${}^7\text{LiH}^+$ ion calculated without the Born–Oppenheimer approximation and with leading relativistic corrections,” *J. Chem. Phys.* **134**, 024103 (2011).
- [50] K. L. Sharkey, S. Bubin, and L. Adamowicz, “Lower Rydberg 2D states of the lithium atom: Finite-nuclear-mass calculations with explicitly correlated Gaussian functions,” *Phys. Rev. A* **83**, 012506 (2011).
- [51] S. Bubin and L. Adamowicz, “Correlated-Gaussian calculations of the ground and low-lying excited states of the boron atom,” *Phys. Rev. A* **83**, 022505 (2011).
- [52] S. Bubin and K. Varga, “First-principles time-dependent simulation of laser assisted desorption of hydrogen atoms from H–Si(111) surface,” *Appl. Phys. Lett.* **98**, 154101 (2011).
- [53] S. Bubin, M. Stanke, and L. Adamowicz, “Complete pure vibrational spectrum of HD calculated without the Born-Oppenheimer approximation and including relativistic corrections,” *Phys. Rev. A* **83**, 042520 (2011).
- [54] K. L. Sharkey, S. Bubin, and L. Adamowicz, “Refinement of the experimental energy levels of higher 2D Rydberg states of the lithium atom with very accurate quantum mechanical calculations,” *J. Chem. Phys.* **134**, 194114 (2011).
- [55] J. A. Driscoll, S. Bubin, W. R. French, and K. Varga, “Time-dependent density functional study of field emission from nanotubes composed of C, BN, SiC, Si, and GaN,” *Nanotechnology* **22**, 285702 (2011).
- [56] J. A. Driscoll, S. Bubin, and K. Varga, “Laser-induced electron emission from nanostructures: A first-principles study,” *Phys. Rev. B* **83**, 233405 (2011).
- [57] S. Bubin and K. Varga, “Ground-state energy and relativistic corrections for positronium hydride,” *Phys. Rev. A* **84**, 012509 (2011).
- [58] J. A. Driscoll, B. Cook, S. Bubin, and K. Varga, “First-principles study of field emission from carbon nanotubes and graphene nanoribbons,” *J. Appl. Phys.* **110**, 024304 (2011).
- [59] S. Bubin, M. Stanke, and L. Adamowicz, “Accurate non-Born-Oppenheimer calculations of the complete pure vibrational spectrum of D_2 with including relativistic corrections,” *J. Chem. Phys.* **135**, 074110 (2011).
- [60] S. Bubin and K. Varga, “Electron-ion dynamics in laser-assisted desorption of hydrogen atoms from H–Si(111) surface,” *J. Appl. Phys.* **110**, 064905 (2011).
- [61] K. L. Sharkey, S. Bubin, and L. Adamowicz, “ 1D states of the beryllium atom: Quantum mechanical nonrelativistic calculations employing explicitly correlated Gaussian functions,” *Phys. Rev. A* **84**, 044503 (2011).
- [62] S. Bubin and L. Adamowicz, “Accurate variational calculations of the ground ${}^2P^o(1s^22s^22p)$ and excited ${}^2S(1s^22s2p^2)$ and ${}^2P^o(1s^22s^23p)$ states of singly ionized carbon atom,” *J. Chem. Phys.* **135**, 214104 (2011).
- [63] S. Bubin and L. Adamowicz, “Explicitly correlated Gaussian calculations of the ${}^2P^o$ Rydberg spectrum of the lithium atom,” *J. Chem. Phys.* **136**, 134305 (2012).
- [64] S. Bubin and K. Varga, “Electron and ion dynamics in graphene and graphene fragments subjected to high-intensity laser pulses,” *Phys. Rev. B* **85**, 205441 (2012).

- [65] S. Bubin, B. Wang, S. Pantelides, and K. Varga, “Simulation of high-energy ion collisions with graphene fragments,” *Phys. Rev. B* **85**, 235435 (2012).
- [66] S. Bubin and L. Adamowicz, “Assessment of the accuracy the experimental energies of the $^1P^o$ $1s^22s6p$ and $1s^22s7p$ states of ^9Be based on variational calculations with explicitly correlated Gaussians,” *J. Chem. Phys.* **137**, 104315 (2012).
- [67] S. Bubin, M. Atkinson, K. Varga, X. Xie, S. Roither, D. Kartashov, A. Baltuška, and M. Kitzler, “Strong laser-pulse-driven ionization and Coulomb explosion of hydrocarbon molecules,” *Phys. Rev. A* **86**, 043407 (2012).
- [68] S. Bubin, M. Pavanello, W.-C. Tung, K. L. Sharkey, and L. Adamowicz, “Born–Oppenheimer and Non-Born–Oppenheimer, Atomic and Molecular Calculations with Explicitly Correlated Gaussians,” *Chem. Rev.* **113**, 36 (2013).
- [69] S. Bubin, A. G. Russakoff, and K. Varga, “Interaction of electromagnetic fields and atomic clusters,” *J. Phys. Conf. Ser.* **436**, 012084 (2013).
- [70] S. Bubin and L. Adamowicz, “Prediction of 2S Rydberg energy levels of ^6Li and ^7Li based on quantum-mechanical calculations performed with explicitly correlated Gaussian functions,” *Phys. Rev. A* **87**, 042510 (2013).
- [71] S. Bubin, K. L. Sharkey, and L. Adamowicz, “Prediction of 2D Rydberg energy levels of ^6Li and ^7Li based on very accurate quantum mechanical calculations performed with explicitly correlated Gaussian functions,” *J. Chem. Phys.* **138**, 164308 (2013).
- [72] J. Mitroy, S. Bubin, W. Horiuchi, Y. Suzuki, L. Adamowicz, W. Cencek, K. Szalewicz, J. Komasa, D. Blume, and K. Varga, “Theory and application of explicitly correlated Gaussians,” *Rev. Mod. Phys.* **85**, 693 (2013).
- [73] S. Bubin, O. V. Prezhdo, and K. Varga, “Instability of tripositronium,” *Phys. Rev. A* **87**, 054501 (2013).
- [74] S. Bubin and O. V. Prezhdo, “Excited States of Positronic Lithium and Beryllium,” *Phys. Rev. Lett.* **111**, 193401 (2013).
- [75] S. Bubin and L. Adamowicz, “Prediction of 1P Rydberg energy levels of beryllium based on calculations with explicitly correlated Gaussians,” *J. Chem. Phys.* **140**, 024301 (2014).
- [76] S. Bubin, M. Stanke, and L. Adamowicz, “Accurate non-Born-Oppenheimer calculations of the complete pure vibrational spectrum of ditritium using all-particle explicitly correlated Gaussian functions,” *J. Chem. Phys.* **140**, 154303 (2014).
- [77] X. Xie, S. Roither, M. Schöffler, H. Xu, S. Bubin, E. Lötstedt, S. Erattupuzha, A. Iwasaki, D. Kartashov, K. Varga, G. G. Paulus, A. Baltuška, K. Yamanouchi, and M. Kitzler, “Role of proton dynamics in efficient photoionization of hydrocarbon molecules,” *Phys. Rev. A* **89**, 023429 (2014).
- [78] K. L. Sharkey, S. Bubin, and L. Adamowicz, “Singlet–triplet energy splitting between 1D and 3D ($1s^2snd$) $n=3,4,5$, and 6, Rydberg states of the beryllium atom (^9Be) calculated with all-electron explicitly correlated Gaussian functions,” *Chem. Phys. Lett.* **616-617**, 254 (2014).
- [79] A. Russakoff, S. Bubin, X. Xie, S. Erattupuzha, M. Kitzler, and K. Varga, “Time-dependent density-functional study of the alignment-dependent ionization of acetylene and ethylene by strong laser pulses,” *Phys. Rev. A* **91**, 023422 (2015).

- [80] S. Bubin, M. Formanek, and L. Adamowicz, “Universal all-particle explicitly-correlated Gaussians for non-Born–Oppenheimer calculations of molecular rotationless states,” *Chem. Phys. Lett.* **647**, 122 (2016).
- [81] S. Bubin and L. Adamowicz, “Lowest 2S Electronic Excitations of the Boron Atom,” *Phys. Rev. Lett.* **118**, 043001 (2017).
- [82] S. Erattupuzha, C. L. Covington, A. Russakoff, E. Lötstedt, S. Larimian, V. Hanus, S. Bubin, M. Koch, S. Gräfe, A. Baltuška, X. Xie, K. Yamanouchi, K. Varga, and M. Kitzler, “Enhanced ionisation of polyatomic molecules in intense laser pulses is due to energy upshift and field coupling of multiple orbitals,” *J. Phys. B* **50**, 125601 (2017).
- [83] S. Bubin, M. Stanke, and L. Adamowicz, “Relativistic corrections for non-Born-Oppenheimer molecular wave functions expanded in terms of complex explicitly correlated Gaussian functions,” *Phys. Rev. A* **95**, 062509 (2017).
- [84] M. Stanke, A. Bralin, S. Bubin, and L. Adamowicz, “Leading relativistic corrections for atomic P states calculated with a finite-nuclear-mass approach and all-electron explicitly correlated Gaussian functions,” *Phys. Rev. A* **97**, 012513 (2018).
- [85] E. M. Chavez, S. Bubin, and L. Adamowicz, “Implementation of explicitly correlated complex Gaussian functions in calculations of molecular rovibrational $J = 1$ states without Born-Oppenheimer approximation,” *Chem. Phys. Lett.* **717**, 147 (2019).