

Publication list of Professor Sándor Suhai

Sándor Suhai

Published online: 15 December 2009
© Springer-Verlag 2009

1. S. Suhai:
Charge carrier mobilities in periodic DNA models,
J. Chem. Phys. **57**, 5599–5603 (1972).
2. S. Suhai and J. Ladik:
The electronic structure of periodic protein models
I. CNDO/2 and MINDO/2 energy band structures of
a two-dimensional formamide network,
Theor. Chim. Acta (Berl.) **28**, 27–35 (1972).
3. P. Greguss, J. Ladik, G. Bizco and S. Suhai:
The effect of electric field on the electronic
structure of DNA II. The G–C base pair in a static
inhomogeneous electric field,
Acta Phys. Hung. **34**, 231–238 (1973).
4. G. Zlatos, M. Járai, S. Suhai, G. Biczó and J. Ladik:
On the ultraviolet absorption spectrum of coen-
zyme B₁₂,
Acta Chim. Hung. **78**, 39–45 (1973).
5. S. Suhai and J. Ladik:
CNDO/2 and MINDO/2 energy band structures of
some homopolynucleotides,
Int. J. Quantum Chem. **7**, 547–560 (1973).
6. S. Suhai:
The electronic structure of periodic protein models
II. Energy band structure and anisotropy of electri-
cal conduction in the parallel-chain β conformation
of polyglycine,
Theor. Chim. Acta (Berl.) **34**, 157–163 (1974).
7. G. Biczó, M. Kertész, I. Lukovits and S. Suhai:
Some remarks on quantum theoretical investiga-
tions on biopolymers and in pharmacology,
Studia Biophysica **46**, 109–113 (1974).
8. S. Suhai and J. Ladik:
Study of the effect of second neighbors' interac-
tions in two-dimensional polypeptide models,
Acta Chim. Hung. **82**, 67–75 (1974).
9. S. Suhai:
Theoretical investigation of semiconductive prop-
erties in proteins. I. Electrical conductivity, charge
carrier mobilities, and free paths in beta-polyglycine,
Biopolymers **13**, 1731–1737 (1974).
10. S. Suhai:
Energy bands and electronic delocalization in the
sugar-phosphate backbone of DNA,
Biopolymers **13**, 1739–1745 (1974).
11. S. Suhai and G. Biczó:
Ab initio and semiempirical band structure calcu-
lation methods for organic semiconductors,
Publications of the Central Research Institute for
Physics of the Hung. Acad. Sci., 109–116 (1974).
12. M. Kertész, S. Suhai and J. Ladik:
PPP DODS crystal orbital calculation of polyene,
polyformamide, polycytosine and poly(s-triazine),
Acta Phys. Hung. **36**, 77–90 (1974).
13. A. Karpfen, J. Ladik, P. Russegger, P. Schuster and
S. Suhai:
Hydrogen bonding in long chains of hydrogen
fluoride and long chains and large clusters of water
molecules,
Theor. Chim. Acta (Berl.) **34**, 115–127 (1974).
14. G. Biczó and S. Suhai:
On the possibility of effective attraction between
delocalized electrons in organic systems,
Physics Letters, **51 A**, 223–225 (1975).
15. S. Suhai:
Bloch- and hopping-type conductivity in polymers
crystals,

S. Suhai (✉)
German Cancer Research Centre, Heidelberg, Germany
e-mail: S.Suhai@dkfz-heidelberg.de

- Publications of the Central Research Institute for Physics of the Hung. Acad. Sci., 245–258 (1975).
16. G. Biczó, M. Kertész und S. Suhai:
Eine neue Methode zur Berechnung der Ladungsverteilung in Polymeren unter Berücksichtigung der Endeffekte,
Zeitschrift für Chemie **15**, 203–204 (1975).
 17. M. Kertész, J. Koller, A. Azman and S. Suhai:
Ab initio energy band structure of polysulfur nitride, poly(SN),
Physics Letters, **55 A**, 107–108 (1975).
 18. S. Suhai, M. Kertész and G. Biczó:
Quantum chemical methods for the investigation of the electronic structure in polymers and molecular crystals,
Chem. Comm. of the Hung. Acad. Sci. **44**, 494–496 (1975).
 19. S. Suhai:
Theoretical investigation of the electrical conductivity in charge transfer molecular crystals of the TCNQ-type,
Chem. Comm. of the Hung. Acad. Sci. **46**, 403–409 (1976).
 20. S. Suhai:
Ground-state electronic properties of the charge transfer molecular crystal NMP-TCNQ: I. One-dimensional treatment including electron correlation,
J. Phys. C: Solid State Phys. **9**, 3073–3086 (1976).
 21. S. Suhai and M. Kertész:
SCF all-valence electron energy band structure of polysulfur nitride,
J. Phys. C: Solid State Phys. **9**, L347–L350 (1976).
 22. M. Kertész, S. Suhai, A. Azman, D. Kocjan and A. I. Kiss:
On the electronic structure of disulfur dinitride: Comments on the applicability of semi-empirical energy band methods for polysulfur nitride,
Chem. Phys. Lett. **44**, 53–57 (1976).
 23. G. Biczó and S. Suhai:
On the role of asymmetry in creating attractive interaction between delocalized electrons of a poly(G–C) DNA model,
Studia Biophysica **55**, 85–92 (1976).
 24. S. Suhai and G. Biczó:
Reduced Coulomb repulsion in NMP-TCNQ through intra- and interchain polarization,
Physics Letters, **62 A**, 380–382 (1977).
 25. S. Suhai, Ch. Merkel and J. Ladik:
Ab initio energy band structure of polycytosine,
Physics Letters, **61 A**, 487–489 (1977).
 26. S. Suhai:
Theoretical estimation of the band- and Coulomb-parameters in K-TCNQ,
Solid State Comm. **21**, 117–120 (1977).
 27. S. Suhai and J. Ladik:
On the electronic properties of the sulfur nitride polymer, poly(SN),
Solid State Comm. **22**, 227–229 (1977).
 28. S. Suhai:
Electron- and phonon-polaron effects in TCNQ,
Physics Letters, **62 A**, 185–188 (1977).
 29. P. Otto, S. Suhai and J. Ladik:
Ab initio supermolecule study of charge transfer in the glyoxal-formamide and in the hydrogensulfid-formamide systems,
Int. J. Quantum Chem.: Quant. Biol. Symp. **4**, 451–457 (1977).
 30. J. Ladik, S. Suhai, P. Otto and T. C. Collins:
Estimation of the band structure of DNA on the basis of an ab initio SCF LCAO band structure of polycytosine,
Int. J. Quantum Chem.: Quant. Biol. Symp. **4**, 55–63 (1977).
 31. J. Ladik, S. Suhai and M. Seel:
Electronic structure of biopolymers and possible mechanism of chemical carcinogenesis,
Int. J. Quantum Chem.: Quant. Biol. Symp. **5**, 35–49 (1978).
 32. S. Suhai, T. C. Collins and J. Ladik:
Theoretical investigation of semiconductive properties in proteins. II. The possibility of charge transfer between proteins and different acceptor molecules,
Biopolymers **18**, 899–908 (1979).
 33. P. G. Mezey, J. Ladik and S. Suhai:
Non-empirical SCF MO studies on the protonation of biopolymer constituents,
Theor. Chim. Acta (Berl.) **51**, 323–329 (1979).
 34. S. Suhai, J. Kaspar and J. Ladik:
Effect of side-chain disorder on the electronic structure of proteins,
Int. J. Quant. Chem. **17**, 995–1006 (1980).
 35. S. Suhai:
A priori electronic structure calculations on highly conducting polymers. I. Hartree–Fock studies on *cis*- and *trans*-polyacetylenes (polyenes),
J. Chem. Phys. **73**(8), 3843–3853 (1980).
 36. S. Suhai:
A priori Hartree–Fock crystal orbital calculations on polydiacetylene backbones,
Chem. Phys. **54**, 91–101 (1980).
 37. S. Suhai and J. Ladik:
Ab initio self-consistent field linear combination of atomic orbitals band structures of infinite TCNQ and TTF stacks,
Physics Letters **77A**, 25–26 (1980).
 38. J. Ladik and S. Suhai:
Ab initio band structure of polycytidine; internal

- charge transfer in DNA,
Int. J. Quant. Chem.: Quant. Biol. Symp. **7**, 181–186 (1980).
39. F. Beleznay, S. Suhai and J. Ladik:
Interaction between polymers: Dispersion energy of two infinite linear chains,
Int. J. Quant. Chem. **20**, 683–692 (1981).
40. J. Ladik, R. D. Singh and S. Suhai:
Calculation of repulsive and effective attractive terms of a sigma-exciton type mechanism for possible superconductivity in polycytosine,
Physics Letters **81A**, 488–490 (1981).
41. R. S. Day, S. Suhai and J. Ladik:
Electronic structure in large finite aperiodic polypeptide chains,
Chemical Physics **62**, 165–169 (1981).
42. S. Suhai and J. Ladik:
Electronic structure of highly conducting polymers,
Mol. Cryst. Liq. Cryst. **85**, 199–210 (1982).
43. P. G. Mezey, G. Del Re, P. Otto, S. Suhai and J. Ladik:
Charge transfer and induced polarization in model peptide-ion complexes,
Int. J. Quant. Chem. **21**, 677–697 (1982).
44. S. Suhai and J. Ladik:
Perturbation theoretical calculation of the correlation energy in an infinite metallic hydrogen chain,
J. Phys. C: Solid State Phys. **15**, 4327–4337 (1982).
45. S. Suhai, P. S. Bagus and J. Ladik:
An error analysis for Hartree–Fock crystal orbital calculations,
Chem. Phys. **68**, 467–471 (1982).
46. A. Imamura, S. Suhai and J. Ladik:
Perturbational approach to the interaction between two nearly incommensurable polymers,
J. Chem. Phys. **76**, 6067–6072 (1982).
47. P. Otto, J. Ladik, G. Corongiu, S. Suhai and W. Förner:
Model calculation of the effect of hydration on the energy band structure of a nucleotide base stack,
J. Chem. Phys. **77**, 5026–5029 (1982).
48. S. Suhai:
Perturbation theoretical investigation of electron correlation effects in infinite metallic and semiconducting polymers,
Int. J. Quant. Chem. **23**, 1239–1256 (1983).
49. S. Suhai:
Bond alternation in infinite polyene: Peierls distortion reduced by electron correlation,
Chem. Phys. Letters **96**, 619–625 (1983).
50. S. Suhai:
Ab initio calculation of polyethylene deformation including electron correlation effects,
J. Polym. Sci.: Polym. Phys. Ed. **21**, 1341–1346 (1983).
51. S. Suhai:
Quasiparticle energy-band structures in semiconducting polymers: Correlation effects on the band gap in polyacetylene,
Phys. Rev. B **27**, 3506–3518 (1983).
52. E. Schwartz, M. Dürst, C. Demankowski, O. Lattermann, R. Zech, E. Wolfsberger, S. Suhai and H. zur Hausen:
DNA sequence and genome organization of genital human papillomavirus Type 6b,
EMBO Journal **2**, 2341–2348 (1983).
53. Y. G. Smeyers, A. Huertas-Cabrera and S. Suhai:
Potential energy calculations for the double internal rotation in acetone and dimethylamine,
Theoret. Chim. Acta (Berl.) **64**, 97–105 (1983).
54. S. Suhai:
Green's function study of optical properties of polymers: Charge-transfer exciton spectra of polydiacetylenes,
Phys. Rev. B **29**, 4570–4581 (1984).
55. S. Suhai:
Electron correlation effects on the mechanical and optical properties of polymers,
Int. J. Quant. Chem.: Quant. Chem. Symp. **18**, 161–171 (1984).
56. S. Suhai:
First principles charge transfer exciton theory of the UV spectrum of DNA,
Int. J. Quant. Chem.: Quant. Biol. Symp. **11**, 223–235 (1984).
57. S. Suhai:
Perturbation theoretical calculation of optical effects in polypeptides,
J. Mol. Struct. **123**, 97–108 (1985).
58. S. Suhai:
Theoretische Berechnung der mikroskopischen, mechanischen und optischen Eigenschaften von Polyäthylen und Polydiazetylen,
Verhandl. der Deutschen Phys. Ges. (VI) **20**, 295–296 (1985).
59. R. M. Flügel, H. Bannert, S. Suhai and G. Darai:
The nucleotide sequence of the early region of the tupaia adenovirus DNA corresponding to the oncogenic region E1b of human adenivirus 7,
Gene **34**, 73–80 (1985).
60. K. Seedorf, G. Krämer, M. Dürst, S. Suhai and W. G. Röwekamp:
Human papillomavirus type 16 DNA sequence,
Virology **145**, 181–185 (1985).
61. A. Imamura, Y. Aoki, S. Suhai and J. Ladik:
Perturbational approach to the interaction between a

- polymer and a small molecule,
J. Chem. Phys. **83**, 5727–5734 (1985).
62. S. Suhai:
Quantum mechanical calculation of the longitudinal elastic modulus and of the deviations from Hooke's law in polyethylene,
J. Chem. Phys. **84**, 5071–5076 (1986).
63. S. Suhai:
On the excitonic nature of the first UV absorption peak in polyene,
Int. J. Quant. Chem. **29**, 469–476 (1986).
64. S. Suhai:
Theory of exciton-photon interaction in polymers:
Polariton spectra of polydiacetylenes,
J. Chem. Phys. **85**, 611–615 (1986).
65. S. Suhai:
Correlation effects on the electronic structure of highly conducting polymers,
Synthetic Metals **17**, 189–196 (1987).
66. J. Reed, W. E. Hull, C.-W. von der Lieth, D. Kübler, S. Suhai and V. Kinzel:
Secondary structure of the Arg–Gly–Asp recognition site in proteins involved in cell-surface adhesion. Evidence for the occurrence of nested β -bends in the model hexapeptide GRGDSP,
Eur. J. Biochem. **178**, 141–154 (1988).
67. S. Suhai:
Computational methods in cancer research: The hierarchy of genomic information,
Interdisc. Science Rev. **14**, 225–232 (1989).
68. S. Suhai:
Bioinformatics aspects of genome research: Current methods and emerging trends,
J. Clin. Chem. Clin. Biochem. **28**, 373–374 (1990).
69. S. Suhai:
The electronic structure of parallel β -pleated sheets in proteins: An ab initio computation including electron correlation,
Int. J. Quant. Chem. **40**, 559–576 (1991).
70. S. Suhai:
On the structure dependence of the static longitudinal linear electric polarizability of infinite polyenes: An *ab initio* uncoupled perturbed Hartree–Fock crystal orbital study,
Molecular Engineering **1**, 115–129 (1991).
71. S. Suhai:
Structural and electronic properties of infinite *cis* and *trans* polyenes: Perturbation theory of electron correlation effects,
Int. J. Quant. Chem. **42**, 193–216 (1992).
72. S. Suhai:
Third-order Møller-Plesset perturbation theory of electron correlation in infinite systems: A comparison of carbon- and silicon-based polymers,
Int. J. Quant. Chem.: Quant. Chem. Symp. **27**, 131–146 (1993).
73. O. Ritter, P. Kocab, M. Senger, D. Wolf and S. Suhai:
Prototype implementation of the integrated genomic database,
Computers and Biomedical Research **27**, 97–115 (1994).
74. S. Suhai:
Electron correlation in extended systems: Fourth-order many-body perturbation theory and density-functional methods applied to an infinite chain of hydrogen atoms,
Phys. Rev. B **50**, 14791–14801 (1994).
75. S. Suhai:
Electron correlation effects in the cohesive properties of ice,
Chem. Phys. Lett. **228**, 471–477 (1994).
76. S. Suhai:
Cooperative effects in hydrogen bonding: Fourth-order many-body perturbation theory studies of water oligomers and of an infinite water chain as a model for ice,
J. Chem. Phys. **101**, 9766–9782 (1994).
77. Y. Aoki, S. Suhai and A. Imamura:
A density functional elongation method for the theoretical synthesis of aperiodic polymers,
Int. J. Quant. Chem. **52**, 267–280 (1994).
78. Y. Aoki, S. Suhai and A. Imamura:
An efficient cluster elongation method in density functional theory and its application to poly-hydrogen-bonding molecules,
J. Chem. Phys. **101**, 10808–10823 (1994).
79. S. Suhai:
Cooperativity and electron correlation effects on hydrogen bonding in infinite systems,
Int. J. Quant. Chem. **52**, 395–412 (1994).
80. M. Kieninger, S. Suhai and I. Mayer:
The chemical Hamiltonian approach in density functional theory,
Chem. Phys. Lett. **230**, 485–490 (1994).
81. M. Kieninger and S. Suhai:
Density functional studies on hydrogen-bonded complexes,
Int. J. Quant. Chem. **52**, 465–478 (1994).
82. F. Herrmann and S. Suhai:
Energy minimization of peptide analogues using genetic algorithms,
J. Comput. Chem. **16**, 1434–1444 (1995).
83. M. Kieniger and S. Suhai:
Computer simulation of antisense DNA containing enantio-deoxynucleotides in the double helix,
Anti-Cancer Drug Design **10**, 189–201 (1995).

84. M. Reczko, A. Hatzigeorgiou, N. Mache, A. Zell and S. Suhai:
A parallel neural network simulator on the connection machine CM-5,
Comp. Appl. in Biosci. (CABIOS) **11**, 309–315 (1995).
85. M. Reczko, A. C. R. Martin, H. Bohr and S. Suhai:
Prediction of hypervariable CDR-H3 loop structures in antibodies,
Protein Engineering **8**, 389–395 (1995).
86. M. Senger, K.-H. Glatting, O. Ritter and S. Suhai:
X-HUSAR, an X-based graphical interface for the analysis of genomic sequences,
Comp. Meth. and Progr. in Biomed. **46**, 131–141 (1995).
87. S. Suhai:
Structure and bonding in the formamide crystal: A complete fourth-order many-body perturbation theoretical study,
J. Chem. Phys. **103**, 7030–7039 (1995).
88. S. Suhai:
Density functional studies of the hydrogen-bonded network in an infinite water polymer,
J. Phys. Chem. **99**, 1172–1181 (1995).
89. S. Suhai:
Electron correlation and dimerization in *trans*-polyacetylene: Many-body perturbation theory versus density-functional methods,
Phys. Rev. B **51**, 16553–16567 (1995).
90. S. Suhai:
Structural and electronic properties of *trans*-polysilene (SiH_x): Many-body perturbation theory versus density-functional methods,
Phys. Rev. B **52**, 1674–1677 (1995).
91. K. J. Jalkanen and S. Suhai:
N-Acetyl-L-alanine *N'*-methylamide: A density functional analysis of the vibrational absorption and vibrational circular dichroism spectra,
Chem. Phys. **208**, 81–116 (1996).
92. M. Kieninger and S. Suhai:
Density functional studies of internal rotation: Formamide as a prototype of the peptide bond,
J. Mol. Struct. **375**, 181–188 (1996).
93. S. Suhai:
Density functional theory of molecular solids: Local versus periodic effects in the two-dimensional infinite hydrogen-bonded sheet of formamide,
J. Phys. Chem. **100**, 3950–3958 (1996).
94. W.-G. Han and S. Suhai:
Density functional studies on *N*-methylacetamide-water complexes,
J. Phys. Chem. **100**, 3942–3949 (1996).
95. O. Ritter, S. Suhai:
Gigabytes über Gigabasen—Informationsintegration in der Genomforschung,
Informationstechnik und Technische Informatik **38**, 16–19 (1996).
96. M. Kieninger and S. Suhai:
Conformational and energetic properties of the ammonia dimer—comparision of post-Hartree–Fock and density functional methods,
J. Comput. Chem. **17**, 1508–1519 (1996).
97. M. Knapp-Mohammady and S. Suhai:
International Symposium on Theoretical and Computational Genome Research,
J. Cancer Res. and Clin. Oncology **122**, 698–701 (1996).
98. I. Mayer, G. Räther and S. Suhai:
The chemical Hamiltonian approach for infinite chains,
Chem. Phys. Lett. **270**, 211–216 (1997).
99. B. Paizs and S. Suhai:
Extension of SCF and DFT versions of the Chemical Hamiltonian Approach to N interacting subsystems and an algorithm for their efficient implementation,
J. Comput. Chem. **18**, 694–701 (1997).
100. G. G. Ferenczy, A. Tóth, I. Bertóti and S. Suhai:
Valence electronic structure of selected polyorganosiloxanes; x-ray photoelectron spectroscopy and quantum chemical studies,
J. Phys.: Condens. Matter **9**, 4781–4790 (1997).
101. E. Tajkhorshid, B. Paizs and S. Suhai:
Conformational effects on the proton affinity of the Schiff Base in Bacteriorhodopsin: A density functional study,
J. Phys. Chem. B **101**, 8021–8028 (1997).
102. J. Karges, O. Ritter and S. Suhai:
Design and implementation of a parallel pipe,
ACM SIGOPS Operating System Review **31**, 60–94 (1997).
103. O. N. Ventura, M. Kieninger, S. Suhai and G. H. F. Diercksen:
The water dimer: Post-Hartree–Fock and density functional calculations on the potential energy surface,
Molecular Engineering **7**, 317–348 (1997).
104. M. Ebeling and S. Suhai:
Molecular databases on the Internet,
J. Mol. Medicine **75**, 620–623 (1997).
105. B. Paizs, S. Suhai:
Comperative study of BSSE correction methods at DFT and MP2 levels of theory,
J. Comput. Chem. **19**, 575–584 (1998).

106. M. Elstner, G. Galli and S. Suhai:
Dynamics of breathers and kink-antikink collisions
in *trans*-polyacetylene studied by an all-valence
electron tight-binding Hamiltonian,
Physica D **113**, 338–341 (1998).
107. G. Halász, Á. Vibók and S. Suhai:
A BSSE-free SCF algorithm for intermolecular
interactions. IV. Generalization for open-shell
systems,
Int. J. Quant. Chem. **68**, 151–158 (1998).
108. I. Mayer, G. Räther and S. Suhai:
Wannier-type orbitals derived from Mulliken's
population analysis,
Chem. Phys. Lett. **293**, 81–89 (1998).
109. M. Kieninger, O. N. Ventura and S. Suhai:
Density functional investigations of carboxyl free
radicals: Formyloxy, Acyloxy, and Benzoyl-
oxy radicals,
Int. J. Quant. Chem., **70**, 253–267 (1998).
110. W.-G. Han, K. J. Jalkanen, M. Elstner and S. Suhai:
Theoretical study of aqueous *N*-Acetyl-L-alanine
N'-Methylamide: Structures and Raman, VCD,
and ROA spectra,
J. Phys. Chem. B **102**, 2587–2602 (1998).
111. M. Kieniger, S. Suhai and O. N. Ventura:
Glycine conformations: gradient-corrected DFT-
studies,
J. Mol. Structure (Theochem) **433**, 193–201
(1998).
112. E. Tajkhorshid, K. J. Jalkanen and S. Suhai:
Structure and vibrational spectra of the zwitterion
L-Alanine in the presence of explicit water mol-
ecules: A density functional analysis,
J. Phys. Chem. B **102**, 5899–5913 (1998).
113. M. Elstner, D. Porezag, G. Jungnickel, J. Elsner,
M. Haugk, Th. Frauenheim, S. Suhai, and G. Seifert:
Self-consistent-charge density-functional tight-
binding method for simulations of complex mate-
rials properties,
Phys. Rev. B **58**, 7260–7268 (1998).
114. M. Senger, T. Flores, K.-H. Glatting, P. Ernst,
A. Hotz-Wagenblatt and S. Suhai:
W2H: WWW interface to the GCG sequence
analysis package,
Bioinformatics **14**, 452–457 (1998).
115. M. Elstner, D. Porezag, G. Jungnickel, T. Frauen-
heim, S. Suhai and G. Seifert:
A Selfconsistent-charge density-functional tight-
binding scheme, in “Tight-Binding Approach
To Computational Materials Science”, Ed.
P. E. A. Turchi, A. Gonis, L. Colombo,
Material Research Society Symp. Proc. **491**, 131–
136 (1998).
116. E. Tajkhorshid and S. Suhai:
Dielectric effects due to the environment on the
structure and proton affinity of retinal Schiff base
models,
Chem. Phys. Lett. **299**, 457–464 (1999).
117. M. Knapp-Mohammady, K. J. Jalkanen, F. Nardi,
R. C. Wade and S. Suhai:
L-alanyl-L-alanine in the zwitterionic state: struc-
tures determined in the presence of explicit water
molecules and with continuum models using
density functional theory,
Chem. Phys. **240**, 63–77 (1999).
118. E. Tajkhorshid and S. Suhai:
The effect of the protein environment on the
structure and charge distribution of the retinal
Schiff base in bacteriorhodopsin,
Theor. Chem. Acc. **101**, 180–185 (1999).
119. Z. W. Luo and S. Suhai:
Estimating linkage disequilibrium between a poly-
morphic marker locus and a trait locus in natural
populations,
Genetics **151**, 359–371 (1999).
120. E. Tajkhorshid, B. Paizs and S. Suhai:
Role of isomerization barriers in the pK_a control of
the retinal Schiff base: A density functional study,
J. Phys. Chem. B **103**, 4518–4527 (1999).
121. B. Paizs, G. Lendvay, K. Vékey and S. Suhai:
Formation of b_2^+ ions from protonated peptides: an
ab initio study,
Rapid Commun. Mass Spectrom. **13**, 525–533 (1999).
122. W.-G. Han, E. Tajkhorshid and S. Suhai:
QM/MM study of the active site of free papain and
of the NMA-papain complex,
J. Biomol. Structure & Dynamics **16**, 1019–1032
(1999).
123. E. Tajkhorshid and S. Suhai:
Influence of the methyl groups on the structure,
charge distribution, and proton affinity of the
retinal Schiff base,
J. Phys. Chem. B **103**, 5581–5590 (1999).
124. P. Hobza, O. Bludsky and S. Suhai:
Reliable theoretical treatment of molecular clus-
ters: Counterpoise-corrected potential energy sur-
face and anharmonic vibrational frequencies of the
water dimer,
Phys. Chem. Chem. Phys. **1**, 3073–3078 (1999).
125. H. G. Bohr, K. J. Jalkanen, M. Elstner, K. Frimand
and S. Suhai:
A comparative study of MP2, B3LYP, RHF and
SCC-DFTB force fields in predicting the vibrational
spectra of *N*-acetyl-L-alanine-*N'*-methyl amide: VA
and VCD spectra,
Chem. Phys. **246**, 13–36 (1999).

126. B. Paizs, E. Tajkhorshid and S. Suhai: Electronic effects on the ground-state rotational barrier of polyene Schiff bases: A molecular orbital study, *J. Phys. Chem. B* **103**, 5388–5395 (1999).
127. M. Elstner, D. Porezag, G. Seifert, Th. Frauenheim and S. Suhai: Selfconsistent-charge density-functional tight-binding method for simulations of biological molecules, in “Multiscale Modelling of Materials”, Ed. T. Diaz de la Rubia, T. Kaxiras, V. Bulatov, N. M. Ghoniem, R. Phillips, *MRS Symp. Proc.* **538**, 541–546 (1999).
128. M. Elstner, Th. Frauenheim, E. Kaxiras, G. Seifert and S. Suhai: A self-consistent charge density-functional based tight-binding scheme for large biomolecules, *Phys. Stat. Sol. (b)* **217**, 357–376 (2000).
129. E. Tajkhorshid, J. Baudry, K. Schulten and S. Suhai: Molecular dynamics study of the nature and origin of retinal’s twisted structure in bacteriorhodopsin, *Biophys. J.* **78**, 683–693 (2000).
130. K. Frimand, H. Bohr, K. J. Jalkanen and S. Suhai: Structures, vibrational absorption and vibrational circular dichroism spectra of L-alanine in aqueous solution: a density functional theory and RHF study, *Chem. Phys.* **255**, 165–194 (2000).
131. Th. Frauenheim, G. Seifert, M. Elstner, Z. Hajnal, G. Jungnickel, D. Porezag, S. Suhai and R. Scholz: A self-consistent charge density-functional based tight-binding method for predictive materials simulations in physics, chemistry and biology, *Phys. Stat. Sol. (b)* **217**, 41–62 (2000).
132. I. P. Csonka, B. Paizs, G. Lendvay and S. Suhai: Proton mobility in protonated peptides: a joint molecular orbital and RRKM study, *Rapid Commun. Mass Spectrom.* **14**, 417–431 (2000).
133. B. Paizs, Z. Szlávík, G. Lendvay, K. Vékey and S. Suhai: Formation of a_2^+ ions of protonated peptides. An ab initio study, *Rapid Commun. Mass Spectrom.* **14**, 746–755 (2000).
134. W.-G. Han, M. Elstner, K. J. Jalkanen, T. Frauenheim and S. Suhai: Hybrid SCC-DFTB/molecular mechanical studies of H-bonded systems and of *N*-Acetyl-(L-Ala)_n *N'*-Methylamide helices in water solution, *Int. J. Quant. Chem.* **78**, 459–479 (2000).
135. E. Tajkhorshid and S. Suhai: The dielectric effect of the environment on the pK_a of the retinal Schiff base and on the stabilization of the ion pair in bacteriorhodopsin, *J. Mol. Struct. (Theochem)* **501–502**, 297–313 (2000).
136. M. Elstner, K. J. Jalkanen, M. Knapp-Mohammady, Th. Frauenheim and S. Suhai: DFT studies on helix formation in *N*-acetyl-(L-alanyl)_n-*N'*-methylamide for $n = 1–20$, *Chem. Phys.* **256**, 15–27 (2000).
137. I. P. Csonka, B. Paizs and S. Suhai: Evaluating the formation of salt-bridges. a molecular orbital study, *Chem. Phys. Lett.* **326**, 129–142, (2000).
138. O. N. Ventura, M. Kieninger, R. E. Cachau and S. Suhai: Density functional computational thermochemistry: determination of the enthalpy of formation of sulfine, $\text{CH}_2=\text{S}=\text{O}$, at room temperature, *Chem. Phys. Lett.* **329**, 145–153 (2000).
139. B. Paizs, J. Baker, S. Suhai and P. Pulay: Geometry optimization of large biomolecules in redundant internal coordinates, *J. Chem. Phys.* **113**, 6566–6572 (2000).
140. T. A. Niehaus, M. Elstner, Th. Frauenheim and S. Suhai: Application of an approximate density-functional method to sulfur containing compounds, *J. Mol. Struct. (THEOCHEM)* **541**, 185–194 (2001).
141. M. Elstner, K. J. Jalkanen, M. Knapp-Mohammady, T. Frauenheim and S. Suhai: Energetics and structure of glycine and alanine based model peptides: Approximate SCC-DFTB, AM1 and PM3 methods in comparison with DFT, HF and MP2 calculations, *Chem. Phys.* **263**, 203–219 (2001).
142. B. Paizs, P. Salvador, A. G. Császár, M. Duran and S. Suhai: Intermolecular bond lengths: extrapolation to the basis set limit on uncorrected and BSSE-corrected potential energy hypersurfaces, *J. Comp. Chem.* **22**, 196–207 (2001).
143. S. W. Bunte, G. M. Jensen, K. L. McNesby, D. B. Goodin, C. F. Chabalowski, R. M. Nieminen, S. Suhai and K. J. Jalkanen: Theoretical determination of the vibrational absorption and Raman spectra of 3-methylindole and 3-methylindole radicals, *Chem. Phys.* **265**, 13–25 (2001).
144. K. J. Jalkanen, R. M. Nieminen, K. Frimand, J. Bohr, H. Bohr, R. C. Wade, E. Tajkhorshid and S. Suhai: A comparison of aqueous solvent models used in the calculation of the Raman and ROA spectra of L-alanine, *Chem. Phys.* **265**, 125–151 (2001).

145. M. Elstner, P. Hobza, T. Frauenheim, S. Suhai and E. Kaxiras:
Hydrogen bonding and stacking interactions of nucleic acid base pairs: A density-functional-theory based treatment,
J. Chem. Phys. **114**, 5149–5155 (2001).
146. P. Salvador, B. Paizs, M. Duran and S. Suhai:
On the effect of the BSSE on intermolecular potential energy surfaces. Comparison of *a priori* and *a posteriori* BSSE correction schemes,
J. Comp. Chem. **22**, 765–786 (2001).
147. B. Paizs, I. P. Csonka, G. Lendvay and S. Suhai:
Proton mobility in protonated glycylglycine and *N*-formylglycylglycinamide: a combined quantum chemical and RRKM study,
Rapid Commun. Mass Spectrom. **15**, 637–650 (2001).
148. B. Paizs and S. Suhai:
Theoretical study of the main fragmentation pathways for protonated glycylglycine, *Rapid Commun. Mass Spectrom.* **15**, 651–663 (2001).
149. T. A. Niehaus, S. Suhai, F. Della Sala, P. Lugli, M. Elstner, G. Seifert and Th. Frauenheim:
Tight-binding approach to time-dependent density-functional response theory,
Phys. Rev. B **63**, 851081–851089 (2001).
150. L. Edler, J. Grassmann and S. Suhai:
Role and results of statistical methods in protein fold class prediction,
Math. and Comp. Modelling **33**, 1401–1417 (2001).
151. H. G. Bohr, K. Frimand, K. J. Jalkanen, R. M. Nieminen and S. Suhai:
Neural-network analysis of the vibrational spectra of *N*-acetyl L-alanyl *N'*-methyl amide conformational states,
Phys. Rev. E **64**, 21905-1–21905-13 (2001).
152. B. Paizs and S. Suhai:
Combined quantum chemical and RRKM modeling of the main fragmentation pathways of protonated GGG. I. *Cis-trans* isomerization around protonated amide bonds,
Rapid Commun. Mass Spectrom. **15**, 2307–2323 (2001).
153. C. Köhler, Z. Hajnal, P. Deák, Th. Frauenheim and S. Suhai:
Theoretical investigation of carbon defects and diffusion in α -quartz,
Phys. Rev. B **64**, 853331–853337 (2001).
154. B. Torralva, T. A. Niehaus, M. Elstner, S. Suhai, Th. Frauenheim and R. E. Allen:
Response of C_{60} and C_n to ultrashort laser pulses,
Phys. Rev. B **64**, 1531051–1531054 (2001).
155. I. P. Csonka, B. Paizs, G. Lendvay and S. Suhai:
Proton mobility and main fragmentation pathways of protonated lysylglycine,
Rapid Commun. Mass Spectrom. **15**, 1457–1472 (2001).
156. A. Bende, Á. Vibók, G. J. Halász and S. Suhai:
BSSE-free description of the formamide dimers,
Int. J. Quant. Chem. **84**, 617–622 (2001).
157. B. Paizs and S. Suhai:
Combined quantum chemical and RRKM modeling of the main fragmentation pathways of protonated GGG. II. Formation of b_2 , y_1 , and y_2 ions,
Rapid Commun. Mass Spectrom. **16**, 375–389 (2002).
158. Th. Frauenheim, G. Seifert, M. Elstner, T. Niehaus, C. Köhler, M. Amkreutz, M. Sternberg, Z. Hajnal, A. Di Carlo and S. Suhai:
Atomistic simulations of complex materials: ground-state and excited-state properties,
J. Phys.: Condens. Matter **14**, 3015–3047 (2002).
159. H. Zhou, E. Tajkhorshid, Th. Frauenheim, S. Suhai and M. Elstner:
Performance of the AM1, PM3, and SCC-DFTB methods in the study of conjugated Schiff base molecules,
Chem. Phys. **277**, 91–103 (2002).
160. C. d. Val, P. Ernst, R. Bräuning, K.-H. Glatting and S. Suhai:
PATH: a task for the inference of phylogenies,
Bioinformatics **18**, 646–647 (2002).
161. B. Paizs, S. Suhai, B. Hargittai, V. J. Hruby and Á. Somogyi:
Ab initio and MS/MS studies on protonated peptides containing basic and acidic amino acid residues. I. Solvated proton vs. salt-bridged structures and the cleavage of the terminal amide bond of protonated RD-NH₂,
Int. J. Mass Spectrom. **219**, 203–232 (2002).
162. B. Paizs and S. Suhai:
Towards understanding some ion intensity relationships for the tandem mass spectra of protonated peptides,
Rapid Commun. Mass Spectrom. **16**, 1699–1702 (2002).
163. S. Abdali, K. J. Jalkanen, H. Bohr, S. Suhai and R. M. Nieminen:
The VA and VCD spectra of various isotopomers of L-alanine in aqueous solution,
Chem. Phys. **282**, 219–235 (2002).
164. G. J. Halász, Á. Vibók, S. Suhai and I. Mayer:
Toward a BSSE-free description of strongly interacting systems,
IJQC **89**, 190–197 (2002).

165. D. Reha, M. Kabelák, F. Ryjácek, J. Sponer, J. E. Sponer, M. Elstner, S. Suhai and P. Hobza: Intercalators. 1. Nature of stacking interactions between intercalators (ethidium, daunomycin, ellipticine, and 4',6-diaminide-2-phenylindole) and DNA base pairs. Ab initio quantum chemical, density functional theory, and empirical potential study, *J. Am. Chem. Soc.* **124**, 3366–3376 (2002).
166. P. Ernst, K.-H. Glatting and S. Suhai: A task framework for the web interface W2H, *Bioinformatics* **19**, 278–282 (2003).
167. A. Bende, M. Knapp-Mohammady and S. Suhai: BSSE-free description of intermolecular force constants in hydrogen fluoride and water dimers, *Int. J. Quant. Chem.* **92**, 152–159 (2003).
168. K. J. Jalkanen, R. M. Nieminen, M. Knapp-Mohammady and S. Suhai: Vibrational analysis of various isotopomers of L-alanyl-L-alanine in aqueous solution: Vibrational absorption, vibrational circular dichroism, Raman and Raman optical activity spectra, *Int. J. Quant. Chem.* **92**, 239–259 (2003).
169. S. Abdali, T. A. Niehaus, K. J. Jalkanen, X. Cao, L. A. Nafie, Th. Frauenheim, S. Suhai and H. Bohr: Vibrational absorption spectra, DFT and SCC-DFTB conformational study and analysis of [Leu]enkephalin, *Phys. Chem. Chem. Phys.* **5**, 1295–1300 (2003).
170. O. V. Shishkin, L. Gorb, A. V. Luzanov, M. Elstner, S. Suhai and J. Leszczynski: Structure and conformational flexibility of uracil: A comprehensive study of performance of the MP2, B3LYP and SCC-DFTB methods, *J. Mol. Struct. (Theochem)* **625**, 295–303 (2003).
171. P. Siedlecki, R. G. Boy, S. Comagic, R. Schirrmacher, M. Wiessler, P. Zielenkiewicz, S. Suhai and F. Lyko: Establishment and functional validation of a structural homology model for human DNA methyltransferase 1, *Biochem. and Biophys. Res. Commun.* **306**, 558–563 (2003).
172. A. Hotz-Wagenblatt, T. Hankeln, P. Ernst, K.-H. Glatting, E. R. Schmidt and S. Suhai: ESTAnnotator: a tool for high throughput EST annotation, *Nuc. Acids Res.* **31**, 3716–3719 (2003).
173. A. Kumar, M. Elstner and S. Suhai: SCC-DFTB-D study of intercalating carcinogens: Benzo(a)pyrene and its metabolites complexed with the G–C base pair, *Int. J. Quant. Chem.* **95**, 44–59 (2003).
174. M. Elstner, T. Frauenheim and S. Suhai: An approximate DFT method for QM/MM simulations of biological structures and processes, *J. Mol. Struct. (Theochem)* **632**, 29–41 (2003).
175. T. Wyttenbach, B. Paizs, P. Barran, L. Breci, D. Liu, S. Suhai, V. H. Wysocki and M. T. Bowers: The effect of the initial water of hydration on the energetics, structures, and H/D-exchange mechanism of a family of pentapeptides: An experimental and theoretical study, *J. Am. Chem. Soc.* **125**, 13768–13775 (2003).
176. Á. Vibók, G. J. Halász, T. Vértesi, S. Suhai, M. Baer and J. P. Toennies: Ab initio conical intersections for the Na+H₂ system: A four-state study, *J. Chem. Phys.* **119**, 6588–6596 (2003).
177. C. del Val, K.-H. Glatting and S. Suhai: cDNA2Genome: A tool for mapping and annotating cDNAs, *BMC Bioinformatics* **4**, 39–46 (2003).
178. B. Paizs, S. Suhai and A. G. Harrison: Experimental and theoretical investigation of the main fragmentation pathways of protonated H-Gly-Gly-Sar-OH and H-Gly-Sar-Sar-OH, *J. Am. Soc. Mass Spectrom.* **14**, 1454–1469 (2003).
179. O. V. Shishkin, M. Elstner, T. Frauenheim and S. Suhai: Structure of stacked dimers of N-methylated Watson–Crick adenine–thymine base pairs, *Int. J. Mol. Sci.* **4**, 537–547 (2003).
180. C. del Val, A. Mehrle, M. Falkenhahn, M. Seiler, K.-H. Glatting, A. Poustka, S. Suhai and S. Wiemann: High-throughput protein analysis integrating bioinformatics and experimental assays, *Nuc. Acids Res.* **32**, 742–748 (2004).
181. T. Crass, I. Antes, R. Basekow, P. Bork, C. Buning, M. Christensen, H. Claußen, C. Ebeling, P. Ernst, V. Gailus-Durner, K.-H. Glatting, R. Gohla, F. Gößling, K. Grote, K. Heidtke, A. Herrmann, S. O’Keefe, O. Kießlich, S. Kolibal, J. O. Korbel, T. Lengauer, I. Liebich, M. van der Linden, H. Luz, K. Meissner, C. von Mering, H.-T. Mevissen, H.-W. Mewes, H. Michael, M. Mokrejs, T. Müller, H. Pospisil, M. Rarey, J. G. Reich, R. Schneider, D. Schomburg, S. Schulze-Kremer, K. Schwarzer, I. Sommer, S. Springstubbé, S. Suhai, G. Thoppae, M. Vingron, J. Warfsmann, T. Werner, D. Wetzel, E. Wingender and R. Zimmer: The Helmholtz Network for Bioinformatics: an integrative web portal for bioinformatics resources, *Bioinformatics* **20**, 268–270 (2004).

182. B. Paizs and S. Suhai:
Towards understanding the tandem mass spectra of protonated oligopeptides. 1: Mechanism of amide bond cleavage,
J. Am. Soc. Mass Spectrom. **15**, 103–113 (2004).
183. K. J. Jalkanen, M. Elstner and S. Suhai:
Amino acids and small peptides as building blocks for proteins: comparative theoretical and spectroscopic studies,
J. Mol. Struct. (Theochem) **675**, 61–77 (2004).
184. I. Mayer, M. Knapp-Mohammady and S. Suhai:
Bond orders and energy components in polymers,
Chem. Phys. Lett. **389**, 34–38 (2004).
185. A. Kumar, M. Knapp-Mohammady, P.C. Mishra and S. Suhai:
A theoretical study of structures and electron affinities of radical anions of guanine–cytosine, adenine–thymine, and hypoxanthine–cytosine base pairs,
J. Comput. Chem. **25**, 1047–1059 (2004).
186. N. Bondar, M. Elstner, S. Fischer, J. C. Smith and S. Suhai:
Can coordinate driving describe proton transfer coupled to complex protein motions?
Phase Transitions **77**, 47–52 (2004).
187. B. Paizs, M. Schnölzer, U. Warnken, S. Suhai and A. G. Harrison:
Cleavage of the amide bond of protonated dipeptides,
Phys. Chem. Chem. Phys. **6**, 2691–2699 (2004).
188. P. Kolandaivel, M. Knapp-Mohammady and S. Suhai:
Studies on structure and conformational stability of free canonical 2'-deoxyribonucleosides: Approximate SCC-DFTB and LMP2 methods,
Int. J. Quant. Chem. **99**, 28–38 (2004).
189. B. Chevreux, T. Pfisterer, B. Drescher, A. J. Driesel, W. E. G. Müller, T. Wetter and S. Suhai:
Using the miraEST assembler for reliable and automated mRNA transcript assembly and SNP detection in sequenced ESTs,
Genome Research **14**, 1147–1159 (2004).
190. A.-N. Bondar, M. Elstner, S. Suhai, J. C. Smith and S. Fischer:
Mechanism of primary proton transfer in bacteriorhodopsin,
Structure **12**, 1281–1288 (2004).
191. M. Baer, T. Vértesi, G. J. Halász, Á. Vibók and S. Suhai:
On diabatization and the topological *D*-matrix: Theory and numerical studies of the H + H₂ system and the C₂H₂ molecule,
Faraday Discuss. **127**, 337–353 (2004).
192. I. P. Csonka, B. Paizs and S. Suhai:
Modeling of the gas-phase ion chemistry of protonated arginine,
J. Mass Spectrom. **39**, 1025–1035 (2004).
193. I. A. Howard, D. J. Klein, N. H. March, C. Van Alsenoy, S. Suhai, Z. Jánosvalfi and Á. Nagy:
Change in electronic structure of polyenes due to interaction with polyacenes and with graphitic strips,
J. Phys. Chem. B **108**, 14870–14875 (2004).
194. A. Vinayagam, R. König, J. Moormann, F. Schubert, R. Eils, K.-H. Glatting and S. Suhai:
Applying Support Vector Machines for Gene ontology based gene function prediction,
BMC Bioinformatics **5**, 116–129 (2004).
195. A. Bende, Á. Vibók, G. J. Halász and S. Suhai:
Ab initio study of the ammonia–ammonia dimer: BSSE-free structures and intermolecular harmonic vibrational frequencies,
Int. J. Quant. Chem. **99**, 585–593 (2004).
196. A.-N. Bondar, S. Fischer, J. C. Smith, M. Elstner and S. Suhai:
Key role of electrostatic interactions in bacteriorhodopsin proton transfer,
J. Am. Chem. Soc. **126**, 14668–14677 (2004).
197. A. N. Bondar, M. Elstner, S. Suhai, S. Fischer and J. C. Smith:
Direct proton transfer in a putative L-state intermediate of the bacteriorhodopsin photocycle,
Phase Transitions **78**, 5–9 (2005).
198. A. Bende, Á. Vibók, G. J. Halász and S. Suhai:
Theoretical study of hydrogen bonds between acetylene and selected proton donor systems,
Int. J. Quant. Chem. **101**, 186–200 (2005).
199. P. C. Mishra, A. K. Singh and S. Suhai:
Interaction of singlet oxygen and superoxide radical anion with guanine and formation of its mutagenic modification 8-oxoguanine,
Int. J. Quant. Chem. **102**, 282–301 (2005).
200. B. Paizs and S. Suhai:
Fragmentation pathways of protonated peptides,
Mass Spectrom. Rev. **24**, 508–548 (2005).
201. A. Bende and S. Suhai:
BSSE-corrected geometry and harmonic and anharmonic vibrational frequencies of formamide–water and formamide–formamide dimers,
Int. J. Quant. Chem. **103**, 841–853 (2005).
202. N. C. Polfer, B. Paizs, L. C. Snoek, I. Compagnon, S. Suhai, G. Meijer, G. von Helden and J. Oomens:
Infrared fingerprint spectroscopy and theoretical studies of potassium ion tagged amino acids and peptides in the gas phase,
J. Am. Chem. Soc. **127**, 8571–8579 (2005).

203. B. Brueckner, R. G. Boy, P. Siedlecki, T. Musch, H. C. Kliem, P. Zielenkiewicz, S. Suhai, M. Wiessler and F. Lyko:
Epigenetic reactivation of tumor suppressor genes by a novel small-molecule inhibitor of human DNA methyltransferases,
Cancer Res. **65**, 6305–6311 (2005).
204. A.-N. Bondar, S. Fischer, S. Suhai and J. C. Smith:
Tuning of retinal twisting in bacteriorhodopsin controls the directionality of the early photocycle steps,
J. Phys. Chem. B Lett. **109**, 14786–14788 (2005).
205. Á. Vibók, G. J. Halász, S. Suhai and M. Baer:
Assigning signs to the electronic nonadiabatic coupling terms: The {H₂O} system as a case study,
J. Chem. Phys. **122**, 1341091–1341098 (2005).
206. A. Kumar, P. C. Mishra and S. Suhai:
Adiabatic electron affinities of the polyhydrated adenine–thymine base pair: A density functional study,
J. Phys. Chem. A **109**, 3971–3979 (2005).
207. N. C. Polfer, J. Oomens, S. Suhai and B. Paizs:
Spectroscopic and theoretical evidence for oxazolone ring formation in collision-induced dissociation of peptides,
J. Am. Chem. Soc. **127**, 17154–17155 (2005).
208. K. J. Jalkanen, V. Würtz-Jürgensen, A. Claussen, A. Rahim, G. M. Jensen, R. C. Wade, F. Nardi, C. Jung, I. M. Degtyarenko, R. M. Nieminen, F. Herrmann, M. Knapp-Mohammady, T. A. Niehaus, K. Frimand and S. Suhai:
Use of vibrational spectroscopy to study protein and DNA structure, hydration, and binding of biomolecules: A combined theoretical and experimental approach,
Int. J. Quant. Chem. **106**, 1160–1198 (2006).
209. Á. Vibók, G. J. Halász, S. Suhai, D. K. Hoffman, D. J. Kouri and M. Baer:
Two-state versus three-state quantization: An ab initio study of the three lower states of the {N, H₂l A'} system,
J. Chem. Phys. **124**, 243121–243128 (2006).
210. P. Siedlecki, R. G. Boy, T. Musch, B. Brueckner, S. Suhai, F. Lyko and P. Zielenkiewicz:
Discovery of two novel, small-molecule inhibitors of DNA methylation,
J. Med. Chem. **49**, 678–683 (2006).
211. A. Vinayagam, C. del Val, F. Schubert, R. Eils, K.-H. Glatting, S. Suhai and R. König:
GOPET: A tool for automated predictions of Gene Ontology terms,
BMC Bioinformatics **7**, 161 (2006) [doi: [10.1186/1471-2105-7-161](https://doi.org/10.1186/1471-2105-7-161)].
212. A. Kumar, P. C. Mishra and S. Suhai:
Binding of gold clusters with DNA base pairs: A density functional study of neutral and anionic GC–Au_n and AT–Au_n ($n = 4, 8$) complexes,
J. Phys. Chem. **110**, 7719–7727 (2006).
213. A. L. Hufton, A. Vinayagam, S. Suhai and J. C. Baker:
Genomic analysis of *Xenopus* organizer function,
BMC Developmental Biology **6**, 27 (2006) [doi: [10.1186/1471-213X-6-27](https://doi.org/10.1186/1471-213X-6-27)].
214. A. G. Harrison, A. B. Young, C. Bleiholder, S. Suhai and B. Paizs:
Scrambling of sequence information in collision-induced dissociation of peptides,
J. Am. Chem. Soc. **128**, 10364–10365 (2006).
215. N. H. March, T. A. Niehaus and S. Suhai:
Influence of the noninteracting density response function on the exchange-only kernel in time-dependent density-functional theory,
Phys. Rev. A **74**, 0445021–0445023 (2006).
216. C. del Val, V. Y. Kuryshov, K.-H. Glatting, P. Ernst, A. Hotz-Wagenblatt, A. Poustka, S. Suhai and S. Wiemann:
CAFTAN: a tool for fast mapping, and quality assessment of cDNAs,
BMC Bioinformatics **7**, 473 (2006) [doi: [10.1186/1471-2105-7-473](https://doi.org/10.1186/1471-2105-7-473)].
217. C. Bleiholder, S. Suhai and B. Paizs:
Revising the proton affinity scale of the naturally occurring α -amino acids,
J. Am. Soc. Mass Spectrom. **17**, 1275–1281 (2006).
218. N. H. March, Zs. Jánosfalvi, Á. Nagy and S. Suhai:
Kinetic and exchange energy related non-locally in Hartree–Fock theory of an inhomogeneous electron liquid,
Phys. & Chem. of Liquids **44**, 493–499 (2006).
219. T. Cooper, E. Talaty, J. Grove, M. Van Stipdonk, S. Suhai and B. Paizs:
Isotope labeling and theoretical study of the formation of a₃^{*} ions from protonated tetraglycine,
J. Am. Soc. Mass Spectrom. **17**, 1654–1664 (2006).
220. N. H. March and S. Suhai:
Can density functional theory make use of experimentally determined ground-state electron densities via the Dirac density matrix for molecules of biological interest?
Phys. Lett. A **360**, 665–668 (2007).
221. A.-N. Bondar, S. Suhai, S. Fischer, J. C. Smith and M. Elstner:
Suppression of the back proton-transfer from Asp85 to the retinal Schiff base in bacteriorhodopsin: A theoretical analysis of structural elements,
J. Struct. Biol. **157**, 454–469 (2007).

222. P. K. Shukla, P. C. Mishra and S. Suhai: Reactions of guanine with methyl chloride and methyl bromide: O6-methylation versus charge transfer complex formation, *Int. J. Quant. Chem.* **107**, 1270–1283 (2007).
223. N. C. Polfer, J. Oomens, S. Suhai and B. Paizs: Infrared spectroscopy and theoretical studies on gas-phase protonated Leu-enkephalin and its fragments: Direct experimental evidence for the mobile proton, *J. Am. Chem. Soc.* **129**, 5887–5897 (2007).
224. C. del Val, P. Ernst, M. Falkenhahn, C. Fladerer, K. H. Glatting, S. Suhai and A. Hotz-Wagenblatt: ProtSweep, 2Dsweep and DomainSweep: protein analysis suite at DKFZ, *Nuc. Acids Res.* **35**, W444–W450 (2007). [doi: [10.1093/nar/gkm364](https://doi.org/10.1093/nar/gkm364)].
225. M. N. Blom, I. Compagnon, N. C. Polfer, G. von Helden, G. Meijer, S. Suhai, B. Paizs and J. Oomens: Stepwise solvation of an amino acid: The appearance of zwitterionic structures, *J. Phys. Chem. A* **111**, 7309–7316 (2007).
226. F. A. Giordano, A. Hotz-Wagenblatt, D. Lauterborn, J.-U. Appelt, K. Fellenberg, K. Z. Nagy, W. J. Zeller, S. Suhai, S. Fruehauf and S. Laufs: New bioinformatic strategies to rapidly characterize retroviral integration sites of gene therapy vectors, *Methods Inf. Med.* **46**, 542–547 (2007).
227. A.-N. Bondar, S. Suhai, J. C. Smith and P. T. Frangopol: Computer simulations of local anesthetics mechanism: Quantum chemical investigation of procaine, *Romanian Reports in Physics* **59**, 289–299 (2007).
228. B. Mersch, N. Sela, G. Ast, S. Suhai and A. Hotz-Wagenblatt: SERpredict: Detection of tissue- or tumor-specific isoforms generated through exonization of transposable elements, *BMC Genetics* **8**, 78 (2007).
229. G. J. Halász, A. Vibók, S. Suhai and M. Baer: The electronic nonadiabatic coupling term: Can it be ignored in dynamic calculations? *J. Chem. Phys.* **127**, 2441011–2441018 (2007).
230. P. K. Shukla, P. C. Mishra and S. Suhai: Reactions of DNA bases with the anti-cancer nitrogen mustard mechlorethamine: A quantum chemical study, *Chem. Phys. Lett.* **449**, 323–328 (2007).
231. N. H. March, S. Suhai and C. C. Matthai: Melting temperature and a precursor phase change in bacteriorhodopsin as function of pH., *Phys. and Chem. of Liquids* **45**, No. 6, 695–699 (2007).
232. K. J. Jalkanen, J. D. Gale, P. R. Lassen, L. Hemmingsen, A. Rodarte, I. M. Degtyarenko, R. M. Nieminen, S. Brøgger Christensen, M. Knapp-Mohammady and S. Suhai: A configurational and conformational study of aframodial and its diastereomers via experimental and theoretical VA and VCD spectroscopies, *Theor. Chem. Account* **119**, 177–190 (2008).
233. S. Tiwari, P. C. Mishra and S. Suhai: Solvent effect of aqueous media on properties of glycine: Significance of specific and bulk solvent effects, and geometry optimization in aqueous media, *Int. J. Quant. Chem.* **108**, 1004–1016 (2008).
234. M. Knapp-Mohammady, N. H. March and S. Suhai: Geometry and ground-state electronic structure of neutral ruthenium metal complexes of potential relevance to metal-based drugs for cancer control, *Phys Lett. A* **372**, 1881–1884 (2008).
235. A. Kumar, M. D. Sevilla and S. Suhai: Microhydration of the guanine-cytosine (GC) base pair in the neutral and anionic radical states: A density functional study, *J. Phys. Chem. B* **112**, 5189–5198 (2008).
236. N. H. March, M. Knapp-Mohammady, C. Van Alsenoy and S. Suhai: Exchange energy density and exchange potential via a hartree–fock plus mp2 study of the electron liquid in the ground-state conformer of glycine, *Phys. and Chem. of Liquids* **46**, 242–254 (2008).
237. B. Mersch, A. Gepperth, S. Suhai and A. Hotz-Wagenblatt: Automatic detection of exonic splicing enhancers (ESEs) using SVMs, *BMC Bioinformatics* **9**:369 (2008).
238. Niehaus, T. A., Suhai, S., and March, N. H.: Dynamical generalization of a solvable family of two-electron model atoms with general interparticle repulsion. *Journal of Physics* **41**(8) (2008).
239. Vaden, T. D., De Boer, T. S. J. A., Simons, J. P., Snoek, L. C., Suhai, S., and Paizs, B.: Vibrational spectroscopy and conformational structure of protonated polyalanine peptides isolated in the gas phase. *Journal of Physical Chemistry A* **112**(20) 4608–4616 (2008).
240. C. Bleiholder, S. Osburn, T. D. Williams, S. Suhai, M. Van Stipdonk, A. G. Harrison, and B. Paizs: Sequence Scrambling Fragmentation Pathways of Protonated Peptides,

- American Chemical Society, **130** (52) 17774–17789 (2008).
241. N. R. Jena, S. Suhai, P. C. Mishra: Protection against radiation induced DNA damage by amino acids: A DFT Study. *The Journal of Physical Chemistry, B* **113** (16) 5633–5644 (2009).
242. P. Phatak, J. Frähmcke, M. Hoffman, P. Strodel, J. Smith, S. Suhai, A.N. Bondar, M. Elsner: Long-distance proton transfer with a break in the bacteriorhodopsin active site *Journal of the American Chemical Society*, **131** (20) 7064–7078 (2009).
243. B. J. Bythell, Á. Somogyi, S. Suhai, and B. Paizs: Proton-driven amide bond cleavage pathways of gas-phase peptide ions lacking mobile protons, *J. Am. Chem. Soc.* **131**, 14057–14065 (2009).
244. C. Bleiholder, S. Suhai, Á. Somogyi, B. Paizs: Fragmentation pathways of doubly protonated tryptic peptides, *J. Am. Soc. Mass Spectrom.*, submitted.