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PREFACE

Preface

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This issue of the Theoretical Chemistry Accounts is dedicated to Professor Fernando Rei Ornellas on the occasion of his 70th birthday. Prof. Ornellas is a theoretical and computational chemist who pioneered the field in Brazil, devoting his career to the study of gas-phase chemistry from first principles and to the formation of the next generations of computational chemists. As part of this celebration, an international scientific conference—Configurating Interactions: Computational Chemistry in São Paulo—CICCSP—was held at the University of São Paulo (USP), Brazil, in the week of July 10–11, 2019. This topical collection contains a selected sample of contributions from his former students, colleagues and collaborators.

After completing a B.S. in Chemistry and a M.Sc. degree in Physical Chemistry at the Institute of Chemistry of the University of São Paulo, Professor Ornellas moved to Bloomington, Indiana, where he had been accepted as a Ph.D. student in the Chemistry Department in 1976, under the supervision of Professor Stanley Hagstrom. After completing his degree requirements, a crucial decision to return to Brazil was made; it was a difficult one because at the time there were not any theoretical/computational chemistry research activities being carried out in Brazilian universities, and worse, the computational infrastructure in the universities was inexistent. By the time of his return, November 1980, the federal university system was chaotic, with most activities paralyzed due to a general strike in the country. It lasted for months. Unexpectedly, after visiting a former member of his Master dissertation committee, Professor José Roberto Leite, at the Department of Condensed Matter, in the Institute of Physics, he learned of a new research institute, latter known as Institute of Advanced Studies—IEAv. This Institute had just been created in the campus of the Aeronautical Technological Center, in São José dos Campos, nearby São Paulo city, and was looking for scientists with a background in atomic and molecular computational physics. They offered him a position as associate researcher, and much to his surprise, they had a slightly better version of the Cyber computer he was using at Indiana University, so he could continue developing his configuration interaction code exactly where he had stopped. At this place, he and his students were able to carry out a series of ab initio calculations for the first time in Brazil. Very soon, a close collaboration with the Institute of Chemistry at the University of São Paulo gave him the opportunity to start his own research group and to teach quantum chemistry in the

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Chemistry Department under the perspective of a quantum chemist. With no senior colleague in the area to consult with, those were years of very difficult decisions and hard work. After a period at the Max-Planck Institut für Astrophysik in Garching, Germany, and a short stay at Indiana University, where Professor Ernst R. Davidson had returned now to chair the Department, Professor Ornellas obtained a copy of the MELD suite of programs which opened the opportunity for his students to carry out ab initio calculations in a routine way when most other incipient groups could only do semiempirical computations. In 1988, he moved full-time to the University of São Paulo as assistant professor; then in 1990, he became associate professor, and in 1992, full professor. In 1995, he spent about 1 year at the Institute for Molecular Science, in Okazaki, Japan, as a visiting professor in the group of Professor Suehiro Iwata.

As a graduate school supervisor, his working motto was "get the right answer for the right reason". With this guiding principle, his students learned to appreciate the effort behind a rigorous calculation and acquire a critical view of the various theoretical approaches. He was very enthusiastic about teaching, especially quantum chemistry, and facing the challenge of having chemistry majors assimilate quantum mechanics concepts and language. He considers his most precious assets to have contributed to the educational and professional supervision of his students, now independent researchers holding academic positions in various institutions.

Besides coordinating the VI Brazilian Symposium of Theoretical Chemistry, in 1991, and committee member in other editions of this symposium, Professor Ornellas acted as an ad hoc advisor for Brazilian and Argentinian funding agencies and several professional journals. He has been a member of the Editorial Board of Theoretical Chemistry Accounts since 2010. He was elected member of the Science Academy of the State of São Paulo in 2012, and Chair of the Department of Fundamental Chemistry in 2009 for a 2-year term, and Director of the Institute of Chemistry from 2010 to 2014.

Aside from his academic life, Professor Ornellas and his wife Emilia enjoy traveling around the world learning about different cultures and exotic places. History and philosophy of religion are also part of his preferred readings. In summary, Professor Ornellas was a strong participant in the process of building and consolidation of the Brazilian theoretical and computational chemistry, staying active as organizing meetings, head of the institutions and patiently mentoring and guiding students. He continues active doing research, teaching and passing his chemistry knowledge with enthusiasm for young students. Besides his numerous academic qualities, we think that everyone who had contact with Professor Ornellas can testify that he is a wonderful human being. In the name of all his students and collaborators, we would like to thank all the authors who contributed to this Festschrift.

Antonio G. S. de Oliveira-Filho, Francisco B. C. Machado, Adélia J. A. Aquino, Ana P. de Lima Batista, Tiago V. Alves, Fernanda Dib Cordeiro
CICCSP Committee

Francisco B. C. Machado
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Guest Editors

1 List of publications of Professor Fernando Rei Ornellas

1. Menezes da Silva VH, Ornellas FR (2020). Spectrochim Acta Part A Mol Biomol Spectrosc 226:117578.
2. dos Santos LG, Ornellas FR (2019). Chem Phys 520:32–39.
3. de Melo GF, Ornellas FR (2019). Chem Phys Lett 722:12–17.
4. Romeu JGF, Ornellas FR (2019). Comput Theor Chem 1158:29–35.
5. de Melo GF, Ornellas FR (2019). J Quant Spectrosc Radiat Transf 237:106632.
6. Romeu JGF, Belinassi AR, Ornellas FR (2018). J Quant Spectrosc Radiat Transf 211:44–49.
7. Gonçalves dos Santos L, Franzreb K, Ornellas FR (2018). J Chem Phys 148:124306.
8. de Melo GF, Ornellas FR (2018). Chem Phys Lett 712:118–122.
9. Stollenwerk PR, Kokish MG, de Oliveira-Filho AGS, Ornellas FR, Odom BC (2018). Atoms 6:53.
10. Belinassi AR, Alves TV, Ornellas FR (2017). Chem Phys Lett 671:78–83.
11. Lins IA, Belinassi AR, Ornellas FR, Alves TV (2017). Chem Phys Lett 682:108–114.
12. Belinassi AR, Ornellas FR (2017). Comput Theor Chem 1115:99–105.
13. de Lima Batista AP, Zahariev F, Slowing II, Braga AAC, Ornellas FR, Gordon MS (2016). J Phys Chem B 120:1660–1669.
14. Alves TV, Simón-Carballido L, Ornellas FR, Fernández-Ramos A (2016). Phys Chem Chem Phys 18:8945–8953.
15. da Silva AGM, Rodrigues TS, Correia VG, Alves TV, Alves RS, Ando RA, Ornellas FR, Wang J, Andrade LH, Camargo PHC (2016). Angew Chemie Int Ed 55:7111–7115.
16. de Lima Batista AP, de Oliveira-Filho AGS, Ornellas FR (2015). Comput Theor Chem 1064:56–61.

17. dos Santos LG, de Oliveira-Filho AGS, Ornellas FR (2015). J Chem Phys 142:024316.
18. da Silva AGM, Rodrigues TS, Wang J, Yamada LK, Alves TV, Ornellas FR, Ando RA, Camargo PHC (2015). Langmuir 31:10272–10278.
19. de Lima Batista AP, Ornellas FR (2015). Surf Sci 641:159–165.
20. de Lima JCB, Alves TV, de Oliveira-Filho AGS, Ornellas FR (2015). Chem Phys Lett 623:22–28.
21. Wang J, Alves TV, Trindade FJ, de Aquino, CB, Pieretti JC, Domingues SH, Ando RA, Ornellas FR, Camargo PHC (2015). Angew Chemie Int Ed 54:14427–14431.
22. de Oliveira-Filho AGS, Ornellas FR, Bowman JM (2014). J Phys Chem A 118:12080–12088.
23. Aoto YA, Ornellas FR (2014). Theor Chem Acc 133:1547.
24. de Lima JCB, Ornellas FR (2014). J Mol Spectrosc 295:1–6.
25. Alves TV, Alves MM, Roberto-Neto O, Ornellas FR (2014). Chem Phys Lett 591:103–108.
26. Alves TV, Ornellas FR (2014). Phys Chem Chem Phys 16:9530–9537.
27. de Oliveira-Filho AGS, Ornellas FR, Bowman JM (2014). J Phys Chem Lett 5:706–712.
28. de Oliveira-Filho AGS, Ornellas FR, Peterson KA (2013). J Chem Phys 139:129901.
29. de Oliveira-Filho AGS, Ornellas FR (2013). J Chem Phys 138:224309.
30. Hermoso W, Jaufeerally NB, Ramasami P, Ornellas FR (2013). Int J Quantum Chem 113:112–118.
31. Ornellas FR, Ramos MJ (2013). Theor Chem Acc 132:1319.
32. de Lima JCB, Ornellas FR (2013). J Mol Spectrosc 283:22–28.
33. Hermoso W, Morf DB, Ornellas FR (2013). J Braz Chem Soc 24:1049–1056.
34. de Lima Batista AP, Ornellas FR (2013). Comput Theor Chem 1009:17–23.
35. Hermoso W, Alves TV, de Oliveira CCS, Moriya E, Ornellas FR, Camargo PHC (2013). Chem Phys 423:142–150.
36. de Oliveira-Filho AGS, Ornellas FR, Peterson KA, Mielke SL (2013). J Phys Chem A 117:12703–12710.
37. de Lima Batista AP, Ornellas FR (2012). Mol Phys 110:3085–3094.
38. Hermoso W, Ornellas FR (2012). Chem Phys 397:98–101.
39. Ornellas FR (2012). Theor Chem Acc 131:1086.
40. de Lima Batista AP, de Lima JCB, Franzreb K, Ornellas FR (2012). J Chem Phys 137:154302.
41. Alves TV, Hermoso W, Ornellas FR, Camargo PHC (2012). Chem Phys Lett 544:64–69.
42. de Lima Batista AP, Ornellas FR (2012). Chem Phys Lett 523:43–48.
43. Hermoso W, Alves TV, Ornellas FR, Camargo PHC (2012). Eur Phys J D 66:135.
44. de Oliveira-Filho AGS, Ornellas FR, Peterson KA (2012). J Chem Phys 136:174316.
45. de Oliveira-Filho AGS, Ornellas FR (2011). Chem Phys Lett 510:31–35.
46. Aoto YA, de Oliveira-Filho AGS, Franzreb K, Ornellas FR (2011). J Chem Phys 134:104303.
47. de Oliveira-Filho AGS, Aoto YA, Ornellas FR (2011). J Chem Phys 135:044308.
48. de Oliveira-Filho AGS, Alves TV, Ribas VW, Ferrão LFA, Roberto-Neto O, Machado FBC (2011). Int J Quantum Chem 111:1694–1700.
49. de Lima Batista AP, de Oliveira-Filho AGS, Ornellas FR (2011). J Phys Chem A 115:8399–8405.
50. Aoto YA, de Oliveira-Filho AGS, Franzreb K, Ornellas FR (2011). J Chem Phys 134:104303.
51. Alves TV, Hermoso W, Ornellas FR (2010). Theor Chem Acc 127:383–391.
52. Hermoso W, Ornellas FR (2010). Chem Phys Lett 499:213–218.
53. Alves TV, Alexandre Aoto Y, Ornellas FR (2010). Mol Phys 108:2061–2071.
54. Hermoso W, Ornellas FR (2010). J Chem Phys 132:194316.
55. Denis PA, Ornellas FR (2009). J Phys Chem A 113:499–506.
56. Hermoso W, Ornellas FR (2009). Chem Phys Lett 479:201–205.
57. Aoto YA, de Oliveira-Filho AGS, Ornellas FR (2009). J Mol Struct Theochem 902:90–95.
58. Ornellas FR (2009). J Phys B At Mol Opt Phys 42:185102.
59. de Oliveira-Filho AGS, Aoto YA, Ornellas FR (2009). J Phys Chem A 113:1397–1402.
60. Hermoso W, Ornellas FR (2009). Quim Nova 32:2487–2491.
61. Denis PA, Ornellas FR (2008). Chem Phys Lett 464:150–154.
62. Ribas VW, Roberto-Neto O, Ornellas FR, Machado FBC (2008). Chem Phys Lett 460:411–416.
63. Ornellas FR (2008). Chem Phys 344:95–100.
64. Hermoso W, Ornellas FR (2008). Chem Phys Lett 459:77–81.
65. Alves TV, de Oliveira-Filho AGS, Ornellas FR (2008). Chem Phys Lett 457:36–41.
66. Aoto YA, Ornellas FR (2007). J Phys Chem A 111:521–5.
67. Ornellas FR (2007). Chem Phys Lett 448:24–30.
68. Ornellas FR (2007). J Chem Phys 126:204314.

69. Roberto-Neto O, Ornellas FR, Machado FBC (2006). Chem Phys Lett 432:403–408.
70. Ueno LT, Machado FBC, Ornellas FR (2006). Chem Phys 321:249–256.
71. Ornellas FR (2006). J Chem Phys 125:114314.
72. Ueno LT, Marim LR, Dal Pino Jr A, Ornellas FR, Machado FBC (2006). Chem Phys Lett 432:11–16.
73. Roberto-Neto O, Machado FBC, Ornellas FR (2005). Chem Phys Lett 409:38–42.
74. Pelegrini M, Vivacqua CS, Roberto-Neto O, Ornellas FR, Machado FBC (2005). Braz J Phys 35:950–956.
75. Roberto-Neto O, Machado FBC, Ornellas FR (2005). Chem Phys 315:27–34.
76. Pelegrini M, Roberto-Neto O, Ornellas FR, Machado FBC (2004). Chem Phys Lett 383:143–148.
77. da Silva-Neto AG, Roberto-Neto O, Ornellas FR, Machado FBC (2004). Chem Phys Lett 395:239–245.
78. Santos LG dos, Ornellas FR (2003). Chem Phys 295:195–203.
79. Resende SM, Ornellas FR (2003). Chem Phys Lett 367:489–494.
80. Resende SM, Ornellas FR (2003). Phys Chem Chem Phys 5:4617.
81. Ornellas FR, Resende SM, Machado FBC, Roberto-Neto O (2003). J Chem Phys 118:4060–4065.
82. Resende SM, Ornellas FR (2002). J Braz Chem Soc 13:565–569.
83. Machado FBC, Resende SM, Ornellas FR (2002). Mol Phys 100:699–704.
84. Ueno LT, Ornellas FR (2001). J Braz Chem Soc 12:99–108.
85. Resende SM, Ornellas FR (2001). Chem Phys Lett 349:123–130.
86. Ueno LT, Ornellas FR (2001). Surf Sci 490:L637–L643.
87. Ornellas FR (2001). Chem Phys Lett 335:420–426.
88. Resende SM, Ornellas FR (2001). J Chem Phys 115:2178–2187.
89. Borin AC, Ornellas FR (2000). Chem Phys Lett 322:149–156.
90. Resende SM, Ornellas FR (2000). Chem Phys Lett 318:340–344.
91. Resende SM, Ornellas FR (2000). J Phys Chem A 104:11934–11939.
92. Ornellas FR, Resende SM (2000). J Phys B At Mol Opt Phys 33:L383–L389.
93. Ornellas FR (2000). Theor Chem Acc 103:469–476.
94. Ornellas FR, Andreazza CM, de Almeida AA (2000). Astrophys J 538:675–683.
95. Singh PD, Sanzovo GC, Borin AC, Ornellas FR (1999). Mon Not R Astron Soc 303:235–238.
96. Machado FBC, Roberto-Neto O, Ornellas FR (1999). Chem Phys Lett 305:156–162.
97. Borin AC, Ornellas FR (1999). Chem Phys 247:351–364.
98. Ornellas FR (1998). Chem Phys Lett 296:25–33.
99. Machado FBC, Roberto-Neto O, Ornellas FR (1998). Chem Phys Lett 284:293–299.
100. Ornellas FR, Iwata S (1998). Chem Phys 232:95–109.
101. Ornellas FR, Borin AC (1998). Mol Phys 94:139–145.
102. Ornellas FR, Borin AC (1998). J Chem Phys 109:2202–2209.
103. Ornellas FR, Iwata S (1997). Chem Phys 107:95–109.
104. Ornellas FR, Ueno LT, Iwata S (1997). J Chem Phys 106:151–157.
105. Ornellas FR, Iwata S (1997). Bull Chem Soc Jpn 70:2057–2062.
106. Ornellas FR, Iwata S (1996). J Phys Chem 100:10919–10927.
107. Ornellas FR, Iwata S (1996). J Phys Chem 100:16155–16161.
108. Borin AC, Ornellas FR (1995). Chem Phys 190:43–52.
109. Borin AC, Ornellas FR (1995). J Mol Struct Theochem 335:107–112.
110. Borin AC, Ornellas FR, Ueno LT (1995). Mol Phys 84:133–140.
111. López-Castillo A, Ornellas FR (1995). Phys Rev A 51:381–390.
112. López-Castillo A, Ornellas FR (1995). Phys Rev A 52:2486–2486.
113. Ornellas FR, Valentim ARS (1994). J Phys Chem 98:12570–12578.
114. Borin AC, Ornellas FR (1994). Chem Phys 184:59–66.
115. Roberto-Neto O, Ornellas FR (1994). J Phys Chem 98:81–87.
116. Roberto-Neto O, Ornellas FR (1994). Chem Phys Lett 226:463–468.
117. Borin AC, Ornellas FR (1993). J Chem Phys 98:8761.
118. Ornellas FR, Machado FBC (1993). J Mol Struct Theochem 282:43–49.
119. Ornellas FR, Machado FBC (1993). J Phys B At Mol Opt Phys 26:1993–2003.
120. Smeyers YG, Ornellas FR, Orville-Thomas WJ (1993). J Mol Struct THEOCHEM 282:vii.
121. Ornellas FR, Machado FBC, Roberto-Neto O (1992). Mol Phys 77:1169–1185.
122. Borin AC, Machado FBC, Ornellas FR (1992). Chem Phys Lett 196:417–421.
123. Ornellas FR, Roberto-Neto O, Borin AC, Machado FBC (1991). J Chem Phys 95:9086–9093.
124. Ornellas FR, Aquino AJA (1991). Theor Chim Acta 79:105–114.
125. Machado FBC, Ornellas FR (1991). J Chem Phys 94:7237–7244.
126. Machado FBC, Ornellas FR (1990). J Mol Struct Theochem 210:259–266.

127. Machado FBC, Ornellas FR (1989). Mol Phys 67:1129–1140.
128. Roberto-Neto O, Ornellas FR (1988). Quim Nova 11: 271–274.
129. Ornellas FR (1987). J Mol Struct Theochem 153:85–91.
130. Ornellas FR, Machado FBC (1986). J Chem Phys 84:1296–1301.
131. Ornellas FR, Olivato PR (1985). Rev Bras Fis 15:87–92.
132. Ornellas FR (1985). J Chem Educ 62:378.
133. Ornellas FR (1985). J Chem Phys 82:379.
134. Rei Ornellas F, Machado FBC (1985). J Mol Struct Theochem 120:149–156.
135. Ornellas FR, Stwalley WC, Zemke WT (1983). J Chem Phys 79:5311–5315.
136. Ornellas FR (1983). J Mol Struct THEOCHEM 92:337–345.
137. Ornellas FR, Hagstrom S (1982). Theor Chim Acta 62:87–92.
138. Ornellas FR (1982). J Phys B At Mol Phys 15:1977–1980.