

# **Spectra Of Charged Solitons And Temperature Dependence Of The Mobility Of Neutral Solitons In Trans-Polyacetylene**

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## **Summary**

On the basis of the dynamics of charged solitons within the Su-Schrieffer-Heeger SSH model geometries of the chain as functions of time are obtained. The SSH model was chosen for the simulation because this one-particle model is based on renormalized parameters that essentially already contain the effects of electron-electron interactions. Furthermore, at least for charged solitons, the theory gives quite correct soliton widths as compared to Pariser-Parr-Pople calculations. Thus the present study is also aimed as a first step to investigate whether the SSH model is really able to yield reliable geometries in time simulations. With the help of the Pariser-Parr-Pople model, Moller-Plesset perturbation theory of second order and the random phase approximation, the spectra as a function of time are calculated at two different doping levels and for an excited chain. Then these spectra calculated at different times are superimposed. All features in the spectra are consistently roughly 0.5 eV too high in energy than expected. Further, the spectra show much more local minima and maxima than the experimental ones. It is suggested that this could be due to a chain length distribution present in the real material. The results show clearly that photogenerated charged solitons appear lower in energy than doping-generated ones and that this effect is not necessarily due to the presence of counterions in the doped material as suggested previously. Further, with the help of explicitly calculated lattice and electron dynamics and again within the Su-Schrieffer-Heeger Hamiltonian, it can be shown that neutral solitons in trans-polyacetylene start to become slightly mobile

from 10 K and completely free above 100 K. This behavior agrees with experimental findings found in the literature. The derivation of equations of motion is given. Further it is shown, that without explicit consideration of electron dynamics the experimental results cannot be reproduced. (C) 2000 John Wiley Sons, Inc.

### References:

1. ABRAMOWITZ A, 1970, HDB MATH FUNCTIONS, P896
2. AMBROSDRAXL C, 1995, PHYS REV B, V51, P9668
3. AMOS AT, 1964, J CHEM PHYS, V41, P1773
4. BAKHSHI AK, IN PRESS SYNTH MET
5. BAKHSHI AK, 1989, SYNTHETIC MET, V30, P115
6. BAKHSHI AK, 1992, ANN REP R SOC C, V89, P147
7. BAKHSHI AK, 1992, SUPERLATTICE MICROST, V11, P465
8. BAKHSHI AK, 1994, INDIAN J CHEM, V13, P494
9. BAKHSHI AK, 1996, J CHEM PHYS, V104, P5528
10. BECKE AD, 1988, PHYS REV A, V38, P3098
11. BECKE AD, 1993, J CHEM PHYS, V98, P5648
12. BISHOP AR, 1984, PHYS REV LETT, V52, P671
13. BLANCHET GB, 1983, PHYS REV LETT, V50, P1938
14. BLANCHET GB, 1983, PHYS REV LETT, V51, P2132
15. BLOCK S, 1996, SYNTHETIC MET, V76, P31
16. BOUDREAUX DS, 1983, PHYS REV B, V28, P6927
17. CEDERBAUM LS, 1973, THEOR CHIM ACTA, V31, P239
18. CEDERBAUM LS, 1977, ADV CHEM PHYS, V36, P205
19. CEDERBAUM LS, 1977, J PHYS B ATOM MOL PH, V10, L549
20. CEDERBAUM LS, 1978, J CHEM PHYS, V69, P1591
21. CRUZEIROHANSSON L, 1992, NANOBIOLOGY, V1, P395
22. CRUZEIROHANSSON L, 1994, PHYS REV LETT, V73, P2927
23. DAVYDOV AS, 1973, PHYS STATUS SOLIDI B, V59, P465
24. DAVYDOV AS, 1979, TEOR MAT FIZ, V40, P408
25. DAVYDOV AS, 1980, ZH EKSP TEOR FIZ+, V78, P789
26. FELDBLUM A, 1982, PHYS REV B, V26, P815
27. FETTER AL, 1971, QUANTUM THEORY MANY
28. FORNER W, 1986, J CHEM PHYS, V84, P5910
29. FORNER W, 1986, SOLID STATE COMMUN, V57, P463
30. FORNER W, 1987, SOLID STATE COMMUN, V63, P941
31. FORNER W, 1988, PHYS REV B, V37, P4567
32. FORNER W, 1989, SYNTHETIC MET, V30, P135
33. FORNER W, 1990, DAVYDOVS SOLITON REV, P267
34. FORNER W, 1991, J PHYS-CONDENS MAT, V3, P4333
35. FORNER W, 1991, PHYS REV B, V44, P11743
36. FORNER W, 1992, CHEM PHYS, V160, P173
37. FORNER W, 1992, CHEM PHYS, V160, P188

38. FORNER W, 1992, J COMPUT CHEM, V13, P275
39. FORNER W, 1992, J PHYS-CONDENS MAT, V4, P1915
40. FORNER W, 1992, NANOBIOLOGY, V1, P413
41. FORNER W, 1992, THESIS U ERLANGEN NU
42. FORNER W, 1993, J MOL STRUCT THEOCHE, V282, P235
43. FORNER W, 1993, J PHYS-CONDENS MAT, V5, P3883
44. FORNER W, 1993, J PHYS-CONDENS MAT, V5, P803
45. FORNER W, 1994, ADV QUANTUM CHEM, V25, P207
46. FORNER W, 1994, J PHYS-CONDENS MAT, V6, P9089
47. FORNER W, 1997, INDIAN J CHEM A, V36, P355
48. FORNER W, 1998, J PHYS-CONDENS MAT, V10, P2631
49. FORNER W, 1998, PHYS SCRIPTA, V58, P640
50. GIBSON HW, 1985, PHYS REV B, V31, P2338
51. GODZIK A, 1986, SOLID STATE COMMUN, V60, P609
52. GRANVILLE MF, 1980, J CHEM PHYS, V72, P4671
53. HARTMANN M, 1996, J LUMIN, V66, P97
54. HARTMANN M, 1996, J LUMINESCENCE, V67
55. HEDIN L, 1969, SOLID STATE PHYS, V23, P1
56. HEEGER AJ, 1983, SOLID STATE COMMUN, V48, P207
57. HEEGER AJ, 1988, REV MOD PHYS, V60, P781
58. HELLER EJ, 1978, J CHEM PHYS, V48, P2067
59. HUDSON BS, 1973, J CHEM PHYS, V59, P4984
60. HUDSON BS, 1982, EXCITED STATES, V6, P1
61. KIVELSON S, 1986, PHYS REV B, V34, P5423
62. KONIG G, 1990, PHYS REV LETT, V65, P1239
63. KOVAR T, 1986, THESIS U ERLANGENNUR
64. LADIK J, 1988, QUANTUM THEORY POLYM
65. LASAGA AC, 1980, J CHEM PHYS, V73, P5230
66. LEE C, 1988, PHYS REV B, V37, P785
67. LIEGENER CM, 1985, J PHYS C SOLID STATE, V18, P6011
68. LIEGENER CM, 1986, CHEM PHYS, V106, P339
69. LIEGENER CM, 1987, PHYS REV B, V35, P6403
70. LIEGENER CM, 1987, SOLID STATE COMMUN, V61, P203
71. LIEGENER CM, 1988, THESIS F ALEXANDER U
72. LINDERBERG J, 1973, PROPAGATORS QUANTUM
73. MAJEWSKI JA, 1992, PHYS REV B, V46, P12219
74. MARKUS R, 1988, SOLID STATE COMMUN, V68, P1
75. MARTINO F, 1970, J CHEM PHYS, V52, P2262
76. MARTINO F, 1971, PHYS REV A, V3, P862
77. MATTUCK RD, 1976, QUIDE FEYNMAN DIAGRA
78. MAYER I, 1973, INT J QUANTUM CHEM, V7, P583
79. MECHTLY B, 1988, PHYS REV B, V38, P3075
80. MOTSCHMANN H, 1989, J PHYS-CONDENS MAT, V1, P5083
81. NAKAHARA M, 1982, PHYS REV B, V25, P7789
82. OHNO K, 1964, THEOR CHIM ACTA, V2, P219

83. OHRN Y, 1976, NEW WORLD QUANTUM CH, P57
84. ORENDI H, 1988, CHEM PHYS LETT, V150, P113
85. ORENSTEIN J, 1982, PHYS REV LETT, V49, P1043
86. PERDEW JP, 1986, PHYS REV B, V33, P8800
87. PHILLPOT SR, 1987, PHYS REV B, V35, P7533
88. ROSENBERG M, 1975, J CHEM PHYS, V63, P5354
89. RUKH R, 1989, J CHEM PHYS, V90, P6463
90. SASAI M, 1984, SYNTHETIC MET, V9, P295
91. SCHINKE R, 1990, J CHEM PHYS, V93, P3252
92. SCHULTEN K, 1972, CHEM PHYS LETT, V14, P305
93. SIMONS J, 1977, ANNU REV PHYS CHEM, V28, P15
94. SKRINJAR MJ, 1988, PHYS REV A, V38, P6402
95. SLATER JC, 1974, QUANTUM THEORY MOL S, V4
96. SOOS ZG, 1983, PHYS REV LETT, V51, P2374
97. SU WP, 1979, PHYS REV LETT, V42, P1698
98. SU WP, 1980, P NATL ACAD SCI USA, V77, P5626
99. SU WP, 1980, PHYS REV B, V22, P2099
100. SU WP, 1980, SOLID STATE COMMUN, V35, P899
101. SU WP, 1986, PHYS REV B, V34, P2988
102. SUHAI S, 1983, PHYS REV B, V27, P3506
103. SUHAI S, 1983, THESIS F ALEXANDER U
104. SUHAI S, 1984, INT J QUANTUM CHEM Q, V11, P223
105. SUHAI S, 1984, PHYS REV B, V29, P4570
106. SUHAI S, 1995, PHYS REV B, V51, P16553
107. SUN JQ, 1996, J CHEM PHYS, V104, P8553
108. SZALAY PG, 1989, CHEM PHYS, V130, P219
109. THOMANN H, 1983, PHYS REV LETT, V50, P533
110. THOMANN H, 1984, SYNTHETIC MET, V9, P255
111. THOMANN H, 1985, J PHYS CHEM-US, V89, P1994
112. THOULESS DJ, 1972, QUANTUM MECH MANY BO
113. UEHARA H, 1980, INT J QUANTUM CHEM, V18, P73
114. VILLAR HO, 1988, J CHEM PHYS, V88, P1003
115. VILLAR HO, 1988, J CHEM PHYS, V88, P5252
116. VILLAR HO, 1988, PHYS REV B, V37, P2520
117. VOSKO SH, 1980, CAN J PHYS, V58, P1200
118. WANG CL, 1986, PHYS REV B, V34, P5540
119. WEINBERGER BR, 1983, PHYS REV LETT, V50, P1693

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