

**J. F. Harrison**  
**Publications from last seven years**

1. "Electronic structure of Li(9-crown-3)<sub>2</sub>: A molecule with a Rydberg-type ground state," R. Rencsok, T. A. Kaplan\*, and J. F. Harrison\*, *J. Chem. Phys.* **98**, 9758 (1993).
2. "Theoretical study of the nonlinear optical properties of KTiOPO<sub>4</sub>: Effects of Ti--O--Ti bond angles and oxygen electronegativity," M. Munowitz\*, R. H. Jarman\*, and J. F. Harrison\*, *Chemistry of Materials* **5**, 1257 (1993).
3. "Magnetism in the insulating parents of the high-T<sub>c</sub> superconductors: Well- or ill-understood," S. D. Mahanti\*, T. A. Kaplan\*, H. Chang, and J. F. Harrison\*, *J. Appl. Phys.* **73**, 6105 (1993).
4. "Theoretical study of the nonlinear optical properties of KTiOPO<sub>4</sub>: Cooperative effects in extended --Ti--O--Ti--O-- Chains," M. Munowitz\*, R. H. Jarman\*, and J. F. Harrison\*, *Chemistry of Materials* **5**, 661 (1993).
5. "Cluster study of the neutron-scattering form factor for antiferromagnetic KNiF<sub>3</sub> and NiO," H. Chang, J. F. Harrison\*, T. A. Kaplan\*, and S. D. Mahanti\*, *Phys. Rev. B* **49**, 15 753 (1994).
6. "An *ab initio* investigation of [111]-cryptates: Their structure and their chemistry," R. C. Boehm, R. J. Rencsok, J. F. Harrison\*, and T. A. Kaplan\*, *J. Phys. Chem.* **98**, 6972 (1994).
7. "Valence-electron distribution of cesium crown-ether electrides," T. A. Kaplan\*, R. Rencsok, and J. F. Harrison\*, *Phys. Rev. B* **50**, 8054 (1994).
8. "Electronic and geometric structure of the diatomics ScN, ScP, and ScAs," F. Tientega and J. F. Harrison\*, *Chem. Phys. Lett.* **223**, 202 (1994).
9. "Electronic and geometric structures of <sup>+</sup>ScSe and <sup>+</sup>ScSeH," J. L. Tilson and J. F. Harrison\*, *J. Phys. Chem.* **98**, 6474 (1994).
10. "Rydberg-like ground states of H[111]-cryptate and H<sub>2</sub>[111]-cryptate: An *ab initio* study," R. C. Boehm, R. J. Rencsok, J. F. Harrison\*, and T. A. Kaplan\*, *J. Phys. Chem.* **98**, 6967 (1994).
11. "Relation of Li(NH<sub>3</sub>)<sub>4</sub> to Electrides," T. A. Kaplan\*, J. L. Dye\*, R. Rencsok, and J. F. Harrison\*, *Phys. Rev. Lett.* **75**, 978 (1995).
12. "Electronic structure of the transition metal nitrides TiN, VN, and CrN," J. F. Harrison\*, *J. Phys. Chem.* **100**, 3513 (1996).
13. "The electronic structure of the neutral, mono and di positive transition metal nitrides, ScN, TiN, VN and CrN," J. F. Harrison\* in *Organometallic Ion Chemistry*, B. S. Freiser, ed., Kluwer Academic: The Netherlands, pp. 89-121 (1995).

14. "Ab initio calculations of ionic and hydrogen bonding interactions with the  $\text{OCN}^-$ ,  $\text{SCN}^-$ , and  $\text{SeCN}^-$  anions," P. W. Schultz, G. E. Leroi\*, and J. F. Harrison\*, *Mol. Phys.* **88**, 217 (1996).
15. "Electronic structures of ScLi, TiLi, VLi, CrLi, and CuLi and their positive ions," D. B. Lawson and J. F. Harrison\*, *J. Phys. Chem.* **100**, 6081 (1996).
16. "Electronic structure of the ground and low-lying excited states of TiP," V. A. Glezakou, A. Mavrides, and J. F. Harrison\*, *J. Phys. Chem.* **100**, 13971 (1996).
17. "A Comprehensive Program for the Enhanced Performance by Minorities in Chemistry at the University Level," D. G. Nocera\*, D. M. Reed, and J. F. Harrison\*, *J. Chem. Ed.* **73**, 1131 (1996).
18. "Electronic properties of the electrone-type molecule  $\text{Li}(9\text{-crown-}3)_2$ ; Comparison of Hartree-Fock and local density approximations," R. Rencsock, K. A. Jackson\*, T. A. Kaplan\*, M. R. Pederson, and J. F. Harrison\*, *Chem. Phys. Lett.* **262**, 207 (1996).
19. "On the Distance Dependence and Spatial Distribution of the Molecular Quadrupole Moments of  $\text{H}_2$ ,  $\text{N}_2$ ,  $\text{O}_2$ , and  $\text{F}_2$ " D. B. Lawson and J. F. Harrison\*, *J. Phys. Chem.* **101**, 4781 (1997).
20. "The Distance Dependence and Spatial Distribution of the Molecular Quadrupole Moments of  $\text{P}_2$ ,  $\text{S}_2$ , and  $\text{Cl}_2$ " D. B. Lawson and J. F. Harrison\*, *Molecular Physics* **93**,519,(1998)
21. "Ab Initio Study of Polycyclic Aromatic Hydrocarbons in their Ground and Excited States" J. V. Goodpaster, J. F. Harrison, and V. L. McGuffin, *J. Phys. Chem.***102**,3372,(1998).
22. "Electronic Structure of the Ground and Low Lying Excited States of CrF and CrCl", J.Hutchison and J. F. Harrison, *Molecular Physics*,**97**, 1009-1027 (1999)
23. "Electronic Structure and Bonding in the Ground and Low Lying Excited States of the Dications  $\text{ScH}^{++}$ ,  $\text{TiH}^{++}$ ,  $\text{VH}^{++}$ ,  $\text{CrH}^{++}$ , and  $\text{MnH}^{++}$ ", J. F. Harrison and P. Christopher. *Molecular Physics* **96**, 31-42 (1999)
28. "Crystal Hartree-Fock Calculations for  $\text{La}_2\text{NiO}_4$  and  $\text{La}_2\text{CuO}_4$  ", Yen-Sheng Su, T. A. Kaplan, S. D. Mahanti, and J. F. Harrison, , *Phys. Rev.* **B59**, 10521, (1999)
29. "Electronic Structure of Diatomic Molecules Composed of a First-Row Transition Metal and Main-Group Element (H-F)" J. F. Harrison, *Chem Rev* **100**, 679-716, (2000)

30. "Electronic Structure of  $\text{LaMnO}_3$  in the ab-initio Crystal Hartree-Fock Approximation", Yen-Sheng Su, T. A. Kaplan, S. D. Mahanti, and J. F. Harrison, *Phys. Rev. B* **61**, 1324, (2000)
31. "Linear Free Energy Relationships for Polyhalogenated Alkane Transformation by Electron Transfer Mediators in Model Aqueous Systems", Judith A. Perlinger, R. Raghuraman and J. F. Harrison, *J. Phys. Chem. A* **2000**, *104*, 2752".
32. "Theoretical Investigation of Scandium Carbide,  $\text{ScC}$ ", A. Kalemou, A. Mavridis, and J. F. Harrison, *J. Phys. Chem A* **2001**, *105*, 755
33. "Comparison of  $\text{CaO}$ ,  $\text{ZnO}$  and  $\text{CaF}_2$ ,  $\text{ZnF}_2$  in their Ground and Low Lying Excited States" J. F. Harrison, R.W. Field, and C. C. Jarrold, A.C.S Symposium on *Accurate Representations of Excited Electronic States*, **In Press**
34. "A Comparison of the Distance Dependence and Spatial Distribution of the Molecular Quadrupole Moments of  $\text{H}_2$ ,  $\text{Li}_2$ , and  $\text{Na}_2$ ", D. B. Lawson and J. F. Harrison, *In Preparation*
35. "Electronic and Geometric Structure of Yttrium Nitride and Yttrium Phosphide in their Ground and Excited States" J.E. Edwards and J.F. Harrison. ***In Preparation***
36. "On the Electronic Structure of  $\text{LiAl}$  in its Ground and Low Lying Excited States", D. B. Lawson and J. F. Harrison, ***In Preparation***.
37. "The Molecular Quadrupole Moments of  $\text{HCCH}$ ,  $\text{FCCF}$ , and  $\text{ClCCl}$ ", D. J. Gearhart and J. F. Harrison, ***In Preparation***
38. "The Molecular Quadrupole Moments of  $\text{CH}_2\text{CH}_2$ ,  $\text{CF}_2\text{CF}_2$  and  $\text{HFCCHF}$ ", B. Papas and J. F. Harrison, ***In Preparation***.