ALICE VEGIRI

PUBLICATIONS – MAY 2009

A. PAPERS IN REFEREED JOURNALS

1. "Ab initio Potential Energy Surfaces of He + OH($X^2\Pi$) and He+OH($A^2\Sigma^+$)", A. Vegiri and S.C. Farantos, J. Phys. Chem. **92**, 2723 (1988).

2. "Quantum Mechanical Study of Rotationally Inelastic Collisions on the He+OH($A^2\Sigma^+$) Excited Potential Energy Surface", S.C. Farantos and A. Vegiri, J. Phys. Chem. **92**, 2719 (1988).

3. "A Classical Dynamical Investigation of the Mechanism of Electronic Quenching of OH($A^2\Sigma^+$) in Collisions with CO", A. Vegiri and S.C. Farantos, Mol. Phys. **69**, 129 (1990).

4. "Ab initio Potential Energy Surfaces for Studying the Quenching of CH($A^2\Delta$) by H_2", A. Vegiri and S.C. Farantos, Chem. Phys. Lett. **167**, 278 (1990).

5. "A Very Efficient and Accurate Charge Control Model for Pseudomorphic Transistors, based on the Variational Technique", G. Halkias, A. Vegiri, G. Pananakakis and A. Christou, Solid-State Electronics **35**, 459 (1992).

6. "Mapping of Transition State Wavefunctions: II A Model for the Photodissociation of ClNO(T1)", A. Vegiri, A. Untch and R. Schinke, J. Chem. Phys. **96,** 3688 (1992).

7. "The photodissociation of ClNO through Excitation of the T1 State: An ab intio Study", D. Solter, H.J. Werner, M. von Dirke, A. Untch, A. Vegiri and R. Schinke, J. Chem. Phys. **97**, 3357 (1992).

8. "Dynamics of Hydrogen-Bonded Systems: Small Water Clusters", A. Vegiri and S.C. Farantos, J. Chem. Phys. **98**, 4059 (1993).

9. "Minimum Structures and Dynamics of Small Water Clusters", S.C. Farantos, S. Kapetanakis and A. Vegiri, J. Phys. Chem. **97**, 12158 (1993).

10. "Quantum Monte-Carlo Studies of Small B(H_2)n Clusters", A. Vegiri, M.H. Alexander, S. Gregurick, A.B. McCoy and R.B. Gerber, J. Chem. Phys. **101**, 2577 (1994).

11. "Flux redistribution during the Photodissociation of ClNO in the T1 state"**,** A. Vegiri and M.H. Alexander, J. Chem. Phys. **101**, 4722 (1994).

12. "Predissociation of the $A^2\Sigma^+$,$C^2\Sigma^+$ and $D^2\Sigma^+$ levels of ^{4}HeH from a multistate close-coupling scattering approach", A. Vegiri and C.A. Nicolaides, J. Phys. B: At. Mol. Opt. Phys. **28**, 2927 (1995).

13. "On the rovibrational spectra of the excimer HeH and its isotopes. A multistate close-coupling treatment", A. Vegiri, J. Phys. B: At. Mol. Opt. Phys. **29**, 3611 (1996).

14. "Theoretical investigation of metastable hydrogen de-excitation in collisions with He and Ne", A. Vegiri, J. Phys. B: At. Mol. Opt. Phys. **31**, 473 (1998).

15. "Device Parameter Optimization of Strained Si Channel SiGe/Si n-MODFET's Using a One- Dimensional Charge Control Model", G. Halkias and A. Vegiri, IEEE Trans. on Electron Devices **45**, 2430 (1998).

16. "Examination of the structural properties of the $H_3O^+(H_2O)_n$ clusters in the (μPT) Grand Canonical ensemble, by employing a new many-body potential energy function", S. V. Shevkunov, and A. Vegiri, J. Chem. Phys. **111,** 9303 (1999).

17. "A revised many-body potential energy function for the description of the $H_3O^+(H_2O)_n$ clusters", S. V. Shevkunov, and A. Vegiri, Mol. Phys. **98**, 149 (2000).

18. "Hydration shell structure of the $OH^-(H_2O)_{n=1-15}$ clusters from a model potential function", A. Vegiri and S. V. Schevkunov**,** J. Chem. Phys. **113**, 8521 (2000).
++Also Virtual Journal of Biological Physics Research, **1**(11).

19. "Cluster Collisions of water tetramers: A classical dynamical study", A. Vegiri and S. C. Farantos, Chem. Phys. **262**, 337 (2000).

20. "Equilibrium Structures of the N=64 Water Cluster in the Presence of External Electric Fields", S. V. Schevkunov and A. Vegiri, J. Mol. Struct., THEOCHEM **574**, 27 (2001).

21. "A Molecular Dynamics Study of Li-doped Borate Glasses", C.P.E. Varsamis, A. Vegiri and E.I.Kamitsos, Cond. Matt. Phys. **4**, 119 (2001).

22. "A Molecular Dynamics Study of Structural Transitions in Small Water Clusters in the Presence of an External Electric Field", A. Vegiri and S. V. Schevkunov, J. Chem. Phys. **115**, 4175 (2001).
++Also Virtual Journal of Biological Physics Research , **2**(9)

23. "Molecular Dynamics Investigation of Lithium Borate Glasses: Local Structures and Ion Dynamics" C.P.E. Varsamis, A. Vegiri and E I. Kamitsos, Phys. Rev. **B65**, 104203 (2002).

24. "Cation Dynamics in Lithium Borate" C.P.E. Varsamis, A. Vegiri and E. I. Kamitsos, J. Non-Cryst. Solids **307-310**, 956 (2002).

25. "Electric Field Induced Transitions in Water Clusters", S. V. Shevkunov and A. Vegiri, J. Mol. Struct., THEOCHEM **593**, 19 (2002).

26. "Translational Dynamics of a Cold Water Cluster in the Presence of an External Uniform Electric Field", A. Vegiri, J. Chem. Phys. **116**, 8786 (2002).
****** Also, Virtual Journal of Biological Physics Research **3**(9).

27. "Reorientational relaxation and rotational-translational coupling in water clusters in a dc external electric field", A. Vegiri, Mol. Liq. **110**, 155 (2004).

28. "Dynamic response of liquid water to an external static electric field at T=250K", A. Vegiri, Mol. Liq. **112**, 107 (2004).

29. "Origin of the enhanced structural and reorientational relaxation rates in the presence of relatively weak dc electric fields", A. Vegiri, Pure Appl. Chem. **76**, 215 (2004).

30. "Clustering and percolation in lithium borate glasses", A. Vegiri and C.P. E. Varsamis, J. Chem. Phys. **120**, 7689 (2004).

31. "The peculiar role of non-bridging oxygen atoms in ionic borate glasses", C.P.E. Varsamis, A. Vegiri and E.I. Kamitsos, Phys. Chem. Glasses **46**, 72 (2005).

32. "Composition- and temperature-dependence of cesium-borate glasses by molecular dynamics", A. Vegiri, C.P.E. Varsamis and E.I. Kamitsos, J. Chem. Phys. **123**, 014508 (2005).

33. "Structure and dynamics of ionic borate glasses", C.P.E. Varsamis, A. Vegiri and E.I. Kamitsos, Phys. Chem. Glasses **47**, 419 (2006).

B. PAPERS IN PROCEEDINGS OF INTERNATIONAL CONFERENCES

1. "Spectroscopic studies of mobile cations in glass", E.I. Kamitsos, C.P.E. Varsamis and A. Vegiri, *Proc. Int. Congr. Glass*, Invited Papers, Edinburgh, Scotland, 2001, Society of Glass Technology, Sheffield, UK, Vol.1, pp 234-246.

C. PAPERS IN PROCEEDINGS OF NATIONAL CONFERENCES (in Greek)

1. "A molecular dynamics study of lithium borate glasses", C.P.E. Varsamis, A. Vegiri

and E.I. Kamitsos, *Proc. XVI Greek Conf. on Solid State Physics*, Nafplion, 2000, pp. 179-182.

2. "Studies of ionic borate glasses by molecular dynamics", C.P.E. Varsamis, A. Vegiri and E.I. Kamitsos, *Proc. XIX Greek Conf. on Solid State Physics*, Thessaloniki, 2003, pp. 609-612.

D. PAPERS IN BOOKS

1. "Electronic Deexcitation of OH($A^2\Sigma^+$) with CO: an ab initio study", A. Vegiri, S.C. Farantos, P. Papagiannakopoulos and C. Fotakis Chemical Reactivity in Excited States, ed. by J.C. Whitehead (Reidel, Dodrecht 1988).