

Invited Presentations

Conferences and Workshops

63. **“P-V-T relations in MgO: an ultrahigh pressure scale for planetary sciences applications”**, American Geophysical Union, Fall07 AGU Meeting, San Francisco, USA (12/07).
62. **“Elasticity of ferropericlase across the spin transition”**, American Geophysical Union, Fall07 Meeting, San Francisco, USA (12/07).
61. **“Elasticity of ferropericlase across the spin transition”**, 2nd *VLab* Workshop, Minneapolis, USA (08/07).
60. **“Spin transition in magnesiowüstite and consequences for elasticity”**, Goldshmidt Conference 2007, (keynote talk) Köln, Germany (08/07).
59. **“Theory of Materials at Ultrahigh Pressures and Temperatures: the Coming of Age of Planetary Materials Science”**, Workshop on Novel Methods in Electronic Structure, Institute for Mathematics and its Applications, Minneapolis, Minneapolis, USA (08/07).
58. **“Spin transition in magnesiowüstite and consequences for elasticity”**, The 16th International Symposium on the Reactivity of Solids, Minneapolis, USA (06/07).
57. **“Theory of materials at ultrahigh pressures and temperatures: the coming of age of planetary materials science”**, EuroMinSci Conference (keynote talk), Nice, France (03/07).
56. **“P-V-T relations in MgO: an ultrahigh pressure scale for planetary sciences applications”**, Workshop on “High Pressure Scales”, Carnegie Institution of Washington, Washington D.C., USA (01/07).
55. **“Theory of Materials at Ultrahigh Pressures and Temperatures: the Coming of Age of Planetary Materials Science”**, American Chemical Society, San Francisco, USA (09/06).
54. **“Minerals at Condition of the Giant’s Interiors”**, General Meeting of the International Mineralogical Association, Kobe, Japan (07/06).
53. **“Spin Transition in Iron Doped Minerals Under Pressure”**, American Ceramics Society, Spring 2006, Baltimore (05/06).
52. **“Spin Transition in Magnesiowüstite Under Pressure”**, Workshop on Synergy of 21st Century High-Pressure Science and Technology, Argonne National Laboratory, USA, (04-05/06).
51. **“Spin Transition in Magnesiowüstite Under Pressure: Elastic Properties”**, American Geophysical Union, Fall05 Meeting, San Francisco, USA (12/05).
50. **“Spin Transition in Magnesiowüstite Under Pressure”**, Workshop on Computational Materials and Molecular Electronics, Austin, USA (10/05).
49. **“MgSiO₃ Post-perovskite at D’ Conditions”**, International Workshop on the Post-Perovskite Phase Transition in the Earth’s Deep Mantle, Tokyo, Japan (10/05).
48. **“MgSiO₃ Post-perovskite at D’ Conditions”**, Earth's Mantle Composition, Structure, and Phase Transitions, Saint-Malo, France (8/05).

47. **“MgSiO₃ Post-perovskite at D” Conditions**”, 1st *Vlab* Workshop, 2005, Minneapolis, USA (7/05).
46. **“The Role of First Principles Calculations in Geophysics”**, Symposium in honor of Marvin Cohen's 70th Birthday, Berkeley, USA (03/05).
45. **“Post-perovskite Transition in MgSiO₃”**, European High Pressure Research Group Annual Meeting ([EHPRG '42](#)), Lausanne, Switzerland (09/04).
44. **“Phase Transition in MgSiO₃ Perovskite in Earth's Lower Mantle”**, [CIDER Workshop](#), Kavli Institute for Theoretical Physics, UC-Santa Barbara, Santa Barbara, USA (07/04).
43. **“Post-perovskite Transition in MgSiO₃”**, [COMPRES Annual Meeting](#), Reno, USA (6/04).
42. **“Thermoelastic Properties of Post-perovskite MgSiO₃”**, [Elasticity Grand Challenge COMRES Meeting](#), Urbana Champaign, USA (5/04).
41. **“Thermoelastic Properties of Post-perovskite MgSiO₃”**, [Joint Assembly AGU, CGU, SEG, EEGS](#), Montreal, Canada (5/04).
40. **“Thermoelasticity of MgSiO₃-perovskite: Consequences for the Inferred Properties of the Lower Mantle”**, [Annual Meeting of the German Mineralogical Society](#) (DMG) (*plenary talk*), Bochum, Germany (9/03).
39. **“Quasiharmonic Thermal Properties of Minerals”**, 15th Annual Workshop on Recent Developments in Electronic Structure Methods (Electronic Structure'03), Minneapolis, USA (5/03).
38. **“Thermoelasticity of MgSiO₃-perovskite at Lower Mantle Conditions”**, Joint Congress of the American Geophysics Union, European Geophysical Society, and European Geophysical Union, Nice, France (4/03).
37. **“Thermoelasticity of MgSiO₃-perovskite at Lower Mantle Conditions”**, [2nd Workshop on Mantle Composition, Structure and Phase Transitions](#), Frejus, France (4/03).
36. **“Theory of Materials at High Pressures and Temperatures”**, NSF-COMPRES workshop, Miami, USA (3/03).
35. **“Thermoelasticity of MgSiO₃-perovskite: Consequences for the Inferred Properties of the Lower Mantle”**, XI International Workshop on Computational Materials Science: Total Energy and Force Methods" at the ICTP, Trieste, Italy (1/03).
34. **“Thermoelasticity of MgSiO₃-perovskite at Lower Mantle Conditions”**, American Geophysics Union, San Francisco, USA (12/02).
33. **“Contrasts and Similarities in Pressure Induced Amorphization”**, CECAM workshop on "Atomic Structure and Transport in Glassy Networks", Lyon, France (6/02).
32. **“Thermoelasticity of MgSiO₃-perovskite at Lower Mantle Conditions”**, Materials Research Society, Spring'02, Symposium on "Perovskite Materials", San Francisco, USA (4/02).
31. **“Optical and Structural Transitions in Ruby: A Tale of Two Oxides”**, CECAM workshop on "Electronic Properties of Strongly Correlated Systems: from the Local Density Approximation to the Dynamical Mean Field Theory", Lyon, France (7/01).
30. **“Optical and Structural Transitions in Ruby: A Tale of Two Oxides”**, CECAM workshop on "Stress-driven Solid-solid Transformation", Lyon, France (7/01).

29. "[Thermoelasticity of Minerals by First Principles](#)", CECAM workshop on "Ab Initio Calculations in Geophysics", Lyon, France (7/01).
28. "**High Pressure and the Earth Mantle**", workshop on "Future Directions in High Pressure Research", organized by Ike Silvera and Bill Nellis, San Francisco, USA (3/01).
27. "[First principles thermoelasticity of mantle minerals](#)", "Mardi Gras Conference on Multiscale Simulation, Theoretical and Experimental Approaches to Deformation, Fatigue, and Fracture", Baton Rouge, USA (2/01).
26. "**First Principles Molecular Dynamics**", Lecture series at the Pan-American Advanced Studies Institute in Computational Materials Science, Santiago, Chile, sponsored by NSF, DOE, and UNESCO (1/01).
25. "**First Principles Thermoelasticity of Minerals**", Gordon Research Conference on Research at High Pressures, New Hampshire. USA (6/00).
24. "**First Principles Thermoelasticity of Minerals: Geophysical Implications**", International Conference on Multiscale Materials Phenomena in Harsh Environments, Limassol, Cyprus (6/00).
23. "**First Principles Thermoelasticity of Minerals: Geophysical Implications**", APS Satellite Meeting. "[Fifteen Years of the Car-Parrinello Method in Physics and Chemistry](#)", Minneapolis, USA (3/00).
22. "**Thermoelasticity of Minerals from First Principles**", [CECAM Workshop on Frontiers in High Pressure Physics](#), Lyon, France (7/99).
21. "**Optical Transitions in Ruby Across the Corundum to Rh₂O₃(II) Transformation**", International Conference on High Pressure Science and Technology, [AIRAPT-17](#), Honolulu, USA (7/99).
20. "**Optical Transitions in Ruby across the Corundum to Rh₂O₃(II) Transformation**", 5th International Conference in Advanced Materials, International Union of Materials Research Societies, Beijing, China (6/99).
19. "**Elasticity of Minerals from First Principles**", APS Centennial Meeting, Atlanta, USA (3/99).
18. "**Silica and Alumina: New Discoveries in Old Systems**", UC-Davis Materials Research Institute Workshop on Electronic Structure, Davis, USA (3/98).
17. "**New Phase and Gradual Coordination Change in Silica Under Pressure**", American Geophysical Union, San Francisco, USA (12/97).
16. "**New Phase and Gradual Coordination Change in Silica Under Pressure**", Materials Research Society, Fall'97, with J. R. Chelikowsky, C. R. S. da Silva, and N. Binggeli, [Symposium on "High Pressure Materials Research"](#) (11/97).
15. "**First Principles Investigation of Elasticity of Earth Materials Under Pressure**", with L. Stixrude (speaker), B. Kiefer, and C. R. S. da Silva, Materials Research Society, Fall'97, [Symposium on "High Pressure Materials Research"](#), (11/97).
14. "**New Phase and Gradual Coordination Change in Silica Under Pressure**", Mardi Gras Conference on "Materials Under Extreme Conditions", Baton Rouge, USA (2/97).
13. "**New Phase and Gradual Coordination Change in Silica Under Pressure**", Workshop on "Computer-Aided Design of High Temperature Materials, Santa Fé, USA (8/97).

12. **"New Phase and Gradual Coordination Change in Silica Under Pressure"**, Adriatico Research Conference on "High Pressure Materials Research: Theory and Experiment", Trieste, Italy (7/97).
11. **"New Phase and Gradual Coordination Change in Silica Under Pressure"**, CECAM Workshop on Mineral Physics, Lyon, France (6/97).
10. **"Pressure Induced Amorphization in BAs: a Possible Inhibited Dissociation"**, Electronic Structure'96, Minneapolis (6/96).
9. **"Ab initio Study of Mantle Minerals at Lower Mantle Pressures"**, with G. D. Price (speaker) and N. Ross, VM Goldschmidt Conference, Edinburgh, UK (9/94).
8. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, [Gordon Research Conference on Structural Phase Transitions](#), Volterra, Italy (5/94).
7. **"Ab initio Molecular Dynamics with Variable Cell Shape: Application to MgSiO₃perovskite"**, American Geophysical Union. San Francisco (12/93).
6. **"Ab initio Study of Mantle Minerals at Lower Mantle Pressures"**, London-Oxford-Cambridge Mineral Physics Symposium, Oxford, UK (11/93).
5. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, Swiss/Italian Workshop on Electronic Structure and Parallel Calculation, Cagliari, Italy (8/93).
4. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, Brazilian Physical Society, Condensed Matter Division, Caxambu, Brazil (5/93).
3. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, APS March Meeting, Seattle USA (3/93).
2. **"Ab initio Molecular Dynamics with Variable Cell Shape: Application to MgSiO₃-perovskite"**, London-Oxford-Cambridge Mineral Physics Symposium, London, UK (11/92).
1. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, Fourth Annual Workshop on Recent Developments in Electronic Structure Methods (Electronic Structure'92), Raleigh. USA (5/92).

Invited talks given by other members of the group

28. **Cesar R. S. da Silva**—"VLab: a service oriented architecture for first principles computations of planetary materials properties", American Geophysical Union, Fall07 AGU Meeting, San Francisco, USA (12/07).
27. **Koichiro Umemoto**—"Spin Transition in ferrous iron in ferrosilicate perovskite", 2nd VLab Workshop, Minneapolis, USA (08/07).
26. **Koichiro Umemoto**—"Ultrahigh pressure forms of ABX₃-type compounds", Workshop of the Center of the Study of Matter at Extreme Conditions, CSMEC, Miami, USA (04/07).
25. **Zhongqing Wu**—"P-V-T relations in MgO: an ultrahigh pressure scale for planetary sciences applications", American Geophysical Union, Fall06 AGU Meeting, San Francisco, USA (12/06).
24. **Koichiro Umemoto**—"Order disorder transition in H₂O self-clathrates", American Geophysical Union, Fall06 AGU Meeting, San Francisco, USA (12/06).

23. *Koichiro Umemoto*—“**Minerals at condition of the giant’s interiors**”, General Meeting of the International Mineralogical Association, Kobe, Japan (07/06).
22. *Koichiro Umemoto*—“**Dissociation of MgSiO₃ in the Gas Giants and in Terrestrial Exoplanets**”, General Assembly, Spring AGU Meeting, Baltimore (2006).
21. *Koichiro Umemoto*—“**Dissociation of MgSiO₃ in the Gas Giants and in Terrestrial Exoplanets**”, Seminar, Department of Physics, U. of Nevada, University, Las Vegas, USA (3/05).
20. *Stefano de Gironcoli* (collaborator from Trieste), “**Spin Transition in Iron Doped Minerals Under Pressure**”, American Physical Society, Baltimore (03/06).
19. *Taku Tsuchiya*—“**Spin Transition in Magnesiowustite in Earth’s Lower Mantle**”, Japan Geosciences Union, Spring06 Meeting, Makuhari, Japan (05/06).
18. *Koichiro Umemoto*—“**Dissociation of MgSiO₃ in the Gas Giants and in Terrestrial Exoplanets**”, American Geophysical Union, Spring06 AGU Meeting, Joint Assembly, Baltimore, USA (05/06).
17. *Koichiro Umemoto*—“**Phase Transformation in MgSiO₃ in the Gas Giants and in Terrestrial Exoplanets**”, American Geophysical Union, Fall05 Meeting, San Francisco, USA (12/05).
16. *Taku Tsuchiya*—“**Post-perovskite Investigated by First Principles**”, American Geophysical Union, Fall05 Meeting, San Francisco, USA (12/05).
15. *Koichiro Umemoto*—“**Dissociation of MgSiO₃ in the Gas Giants and in Terrestrial Exoplanets**”, Condensed Matter Physics Seminar, Department of Physics, Stony Brook University, Stony Brook, USA (11/05).
14. *Koichiro Umemoto*—“**Dissociation of MgSiO₃-post-perovskite: Significance for the Solar Giants and Exoplanets**”, International Workshop on the Post-Perovskite Phase Transition in the Earth’s Deep Mantle, Tokyo, Japan (10/05).
13. *Taku Tsuchiya*—“**Spin Transition in Magnesiowustite in Earth’s Lower Mantle**”, International Workshop on the Post-Perovskite Phase Transition in the Earth’s Deep Mantle, Tokyo, Japan (10/05).
12. *Koichiro Umemoto*—“**Dissociation of MgSiO₃-post-perovskite: Significance for the Solar Giants and Exoplanets**”, 1st *Vlab* Workshop, 2005, Minneapolis, USA (7/05).
11. *Taku Tsuchiya*—“**Spin Transition in Magnesiowustite in Earth’s Lower Mantle**”, 1st *Vlab* Workshop, 2005, Minneapolis, USA (7/05).
10. *Taku Tsuchiya*—“**MgSiO₃ Post-Perovskite at D” conditions**”, [Goldschmidt Conference 2005](#), Moscow, USA (5/05).
9. *Taku Tsuchiya*—“**MgSiO₃ Post-Perovskite at D” conditions**”, American Geophysical Union, [2004 Fall Meeting](#), San Francisco, USA (12/04).
8. *Taku Tsuchiya*—“**Post-Perovskite Transition in MgSiO₃**”, American Geophysical Union, Montreal, Canada (05/04).
7. *Koichiro Umemoto*—“**Low ↔ High Density Transformations in H₂O-ice**”, American Geophysical Union, San Francisco, USA (12/03).

6. **Koichiro Umemoto**—“**Low ↔ High Density Transformations in H₂O-ice**”, [IUCr/COMPRES High Pressure Workshop](#), Berkeley, USA (12/03).
5. **Koichiro Umemoto**—“**Amorphization and Other Pressure Induced Anomalies in H₂O-ice**”, 15th Annual Workshop on Recent Developments in Electronic Structure Methods ([Electronic Structure '03](#)), Minneapolis, USA (5/03).
4. **Bijaya B. Karki**—“**Thermoelastic Properties of Mantle Minerals and Geophysical Implications**”, Mardi Gras Conference on Multiscale Simulation, Theoretical and Experimental Approaches to Deformation, Fatigue, and Fracture, Baton Rouge, USA (2/01).
3. **Bijaya B. Karki**—“**First Principles Thermoelasticity of Minerals**”, XIX European Crystallographic Meeting. Symposium on Theoretical Studies of Minerals and Minerals' Properties, Nancy, France (8/00).
2. **Bijaya B. Karki**—“**First Principles Thermoelasticity of Minerals: Geophysical Implications**”, XXXI International Geological Congress, Symposium on Physics and Chemistry of Minerals, Rio de Janeiro, Brazil (8/00).
1. **Bijaya B. Karki**—“**First Principles Thermoelasticity of Minerals: Geophysical Implications**”, Twelfth Annual Workshop on Recent Developments in Electronic Structure Methods ([Electronic Structure 2000](#)), Atlanta, USA (5/00).

Seminars

48. “**Elasticity of ferropericlase across the spin transition**”, Department of Electrical Engineering, U. Minnesota, Minneapolis, USA (10/07).
47. “**Invariant Molecular Dynamics Approach to Structural Phase Transition**”, Department of Physics, Tokyo Institute of Technology, Tokyo, Japan (07/06).
46. “**Advances and Challenges in the Theory of Planetary Materials**”, Department of Physics, Tokyo Institute of Technology, Tokyo, Japan (07/06).
45. “**Spin transition in Magnesiowustite in Earth’s mantle**”, Department of Earth and Planetary Sciences, Tokyo Institute of Technology, Tokyo, Japan (07/06).
44. “**Advances and Challenges in the Theory of Planetary Materials**”, Seminar at the Department of Physics, University of Nevada, Las Vegas, USA (3/06).
43. “**Advances and Challenges in the Theory of Planetary Materials**”, Colloquium at the Department of Physics and Astronomy, University of Minnesota, Minneapolis, USA (2/06).
42. “**Advances and Challenges in the Theory of Planetary Materials**”, Colloquium at the Department of Physics and Astronomy, Stony Brook University, Stony Brook, USA (11/05).
41. “**Spin transition in Iron Doped Minerals**”, Institute for the Theory of Advanced Material in Information Technology, U. of Minnesota, Minneapolis, USA (07/05).
40. “**MgSiO₃ Post-Perovskite at D” Conditions**”, Department of Earth, Atmospheric, and Planetary Sciences, MIT, Boston (4/05).

39. **“MgSiO₃ Post-Perovskite at D” Conditions**”, SUNY-Stony Brook, Department of Geosciences, SUNY-Stony Brook, Stony Brook, USA (1/05).
38. **“MgSiO₃ Post-Perovskite at D” Conditions**”, Department of Geosciences, University of Chicago, Chicago, USA (1/05).
37. **“Phase Transition in MgSiO₃ Perovskite in Earth’s Lower Mantle”**, [DEMOCRITOS National Simulation Center](#), SISSA, Trieste, Italy (8/04).
36. **“Composition Controlled Spin Polarization in Co_{1-x}Fe_xS₂”**, Institute for the Theory of Advanced Material in Information Technology, U. of Minnesota, Minneapolis, USA (7/04).
35. **“Thermoelasticity of MgSiO₃-perovskite: Consequences for the Inferred Properties of the Lower Mantle”**, [Seismology Laboratory, Harvard University](#), Boston, USA (11/02).
34. **“Thermoelastic Properties of Lower Mantle Minerals”**, Umbgrove Lecture, Faculty of Geosciences, University of Utrecht, Holland (5/04).
33. **“Thermoelasticity of MgSiO₃-perovskite: Consequences for the Inferred Properties of the Lower Mantle”**, Department of Earth and Planetary Sciences, Washington University, Saint Louis, USA (11/02).
32. **“Thermoelasticity of Minerals from First Principles”**, [Department of Geology, University of Illinois, Urbana-Champaign](#), USA (11/02).
31. **“Thermoelasticity of Minerals from First Principles”**, [Department of Physics, Ohio State University](#), Columbus, USA (10/02).
30. **“Thermoelasticity of Minerals from First Principles”**, [Department of Geosciences, Princeton University](#), Princeton, USA (9/02).
29. **“Thermoelasticity of Minerals from First Principles”**, [Department of Geological Sciences, University College London](#), London, UK (9/02).
28. **“Thermoelasticity of Minerals from First Principles”**, International Center for Theoretical Physics, Trieste, Italy (5/02).
27. **“First Principles Calculations in Mineral Physics”**, [Department of Physics, Tokyo Institute of Technology](#), Tokyo, Japan (3/02).
26. **“First Principles Thermoelasticity of Minerals”**, [Department of Earth and Planetary Sciences, Tokyo Institute of Technology](#), Tokyo, Japan (3/02).
25. **“Materials Theory and Mineral Physics”**, seminar speaker, [Institute of Geophysics and Planetary Physics, UCLA](#), Los Angeles (5/01).
24. **“First Principles Thermoelasticity of Minerals: Applications to Mantle Minerals”**, Department of Earth Sciences, U. of Cambridge, Cambridge, UK (11/00).
23. **“First Principles Thermoelasticity of Minerals: Applications to Mantle Minerals”**, Colloquium speaker at the Department of Physics, University of Colorado, Boulder, CO (4/00).
22. **“First Principles Thermoelasticity of Minerals: Applications to Mantle Minerals”**, Colloquium speaker at the Department of Physics, SUNY-Stony Brook, NY (11/99).
21. **“New Phase and Gradual Coordination Change in Silica Under Pressure”**, Department of Physics (Condensed Matter Group), SUNY-Stony Brook, NY (8/97).

20. **"First Principles Studies of Minerals Under Pressure"**, Department of Physics (Condensed Matter Group), SUNY-Stony Brook, NY (2/96).
19. **"First Principles Studies of Minerals Under Pressure"**, Department of Physics, Univ. of Coimbra, Portugal (1/96).
18. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, Department of Materials Physics. Univ. of São Paulo, Brazil (11/95).
17. **"Ab initio Molecular Dynamics with Variable Cell Shape: Applications to MgSiO₃-perovskite and VO₂"**, Department of Physics, Univ. of Minnesota (7/95).
16. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, Department of Geology and Geophysics, Univ. of Minnesota (7/95).
15. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, Cray Research, Eagan, MN (1/95).
14. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, Department of Physics (Cond. Matter Group), Univ. of Minnesota, (11/94).
13. **"Ab initio Molecular Dynamics with Variable Cell Shape: Applications to MgSiO₃-perovskite and VO₂"**, Max-Planck Institut, Stuttgart, Germany (5/94).
12. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, Department of Physics, Keele, UK (5/94).
11. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, Department of Physics, Aarhus, Denmark (5/94).
10. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, Department of Physics, Bristol, UK (5/94).
9. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, Department of Materials Sciences, Oxford, UK (5/94).
8. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, Department of Chemical Engineering and Materials Sciences, University of Minnesota, Minneapolis. USA (5/94).
7. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, Department of Physics, Daresbury Laboratory, UK (2/94)
6. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, Department of Solid State Physics, Univ. of Campinas, Campinas, Brazil (8/93).
5. **"Ab initio Molecular Dynamics with Variable Cell Shape: Application to MgSiO₃-perovskite"**, Laboratoire de Physique des Milieu Condenses Pierre et Marie Curie, Paris (6/93).
4. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, The Royal Institution of Great Britain, Michael Faraday Laboratory. London (5/93).
3. **"Ab initio Molecular Dynamics with Variable Cell Shape: Application to M₉SiO₃-perovskite"**, Department of Physics, Brookhaven National Laboratory, Upton, NY (3/93).
2. **"Ab initio Molecular Dynamics with Variable Cell Shape: Applications to M₉SiO₃-perovskite and VO₂"**, Fritz-Haber Institut, Berlin, Germany (2/93).
1. **"Ab initio Molecular Dynamics with Variable Cell Shape"**, Cavendish Laboratory, Cambridge. UK (10/92).