CURRICULUM VIAE

1. Personal Details

Name:	Peijun Hu
Date of birth:	8 August, 1957
Sex:	Male
Marital Status:	Married

2. Education

1989-93	Ph.D.	University of Cambridge, UK
1982-85	M.S.	East China University of Science and Technology, China
1978-82	B.S.	East China University of Science and Technology, China

3. Experience

2004-	Professor	The Queen's University of Belfast
2001-2004	Reader	The Queen's University of Belfast
1995-2001	Lecturer	The Queen's University of Belfast
1993-1995	Post-Doctoral Research Associate	University of Cambridge
1988-89	Visiting Scientist	University of Cambridge
1985-88	Lecturer	East China University of Science and Technology

4. Some highlights

4.1. Publications in top journals: two in **Nature**, four in **Phys. Rev. Letters**, thirteen in **J. Am. Chem. Soc.**.

4.2. Both the total citation number and citation/paper are highest in heterogeneous catalysis and surface science in the UK in the last few years.

4.3. My group have received several national and international awards: Best Ph.D. thesis in Chemical Sciences in Ireland (1999, 2003); IUPAC Prize for Young Chemists (2004); IUPAC Honourable Mention Award (2000).

Invited talks in conferences and seminars

42. Invited talk at
Beijing University
28 July, 2005

41. Invited talk at
East China University of Science and Technology
21 July, 2005

40. Invited talk at
Fudan University
20 July, 2005

39. Invited speaker at
Interdisciplinary Surface Science Conference 15
Cardiff
27-30 June, 2005

38. Invited speaker at
7th Congress of the World Association of Theoretically Oriented Chemists,
Cape Town
16-21 January, 2005

37. Invited talk at
Fritz-Haber-Institut, Berlin
10 Feb., 2005

36. Invited talk at
3th Taylor International Conference
Belfast, UK
6 – 8 September, 2004

35. Invited talk at
East China University of Science and Technology
12 August, 2004

34. Invited talk at
Dalian Institute of Chemical Physics
5 August, 2004

33. Invited talk at
Institute of Metal Research, Shenyang
28 July, 2004

32. Invited talk at
Fudan University
24 July, 2004

31. Invited talk at
International Conference on Atomistic Simulation
Belfast, UK
21 May, 2004

30. Invited talk at
Johnson Matthey, UK
18 May, 2004

29. Invited talk at
Fudan University
29 November, 2003

28. Invited talk at
International Workshop in Computational Materials Physics
Taiwan
22 November, 2003

27. Invited talk at
Workshop on Advanced Materials Science
Taiwan
20-21 November, 2003

26. Invited talk at
26^{th} American Chemical Society National Meeting
New York
7-11 September, 2003

25. Invited talk at
Aarhus University
11 February, 2003

24. Invited talk at
Royal Society of Chemistry, Theoretical Chemistry Group Meeting
University College London
London
4 December, 2002

23. Invited talk at
University College London
London
4 November, 2002

22. Invited talk at
Technical University of Denmark
Lyngby, Denmark
5 September, 2002

21. Invited talk at
Xiamen University
15 July, 2002

20. Invited talk at
Fudan University
12 July, 2002

19. Invited talk at
University of Cambridge
5 June, 2002

18. Invited talk at
Rideal Conference
Manchester, UK
March 2002

17. Invited talk at
3rd workshop on “Catalysis from first principles”
Vienna, Austria
Feb., 2002

16. Invited talk at
Applied Math and Physics, QUB
29 January, 2002

15. Invited talk at
5th European Conference on Catalysis
Limerick, Ireland,
September, 2001

14. Invited talk at
5th Workshop on Gas Surface Interactions,
Innsbruck, Austria,
May, 2001

13. Invited talk at
“Can Theoretical Catalysis Describe Reality?”,
Liverpool, UK
September, 2000

12. Invited talk at
Fudan University
July, 2000

11. Invited talk at
8th International conference on Theoretical Aspects of Heterogeneous Catalysis
La Colle sur Loup, France
May, 2000

10. Invited talk at
A Symposium on Reactive Surfaces
Cambridge, UK
September, 1999

9. Invited talk at
Trinity College,
Dublin, Ireland
November 1999

8. Invited talk at
Tamkang University, Taiwan,
June, 1999

7. Invited talk at
Dublin City University,
Dublin, Ireland
May 1996

6. Invited talk at
Rideal Conference
Dundee, UK
March, 1996

5. Invited talk at
University of Cambridge, UK
November, 1995

4. Invited talk at
Ivth European Conference on Surface Crystallography,
Aarhus, Denmark
May, 1993

3. Invited talk at
ESF/CCP3 Workshop on Low Energy Electron Diffraction,
Cambridge, UK
March, 1993

2. Invited talk at
ESF Workshop on Holographic and Local Diffraction at Surfaces II,
Madrid, Spain
September, 1992

1. Invited talk at
ESF Workshop on Holographic and Local Diffraction at Surfaces I,
Warwick, UK.
April, 1991

Publications

81. B. McAllister and P. Hu: "A Density Functional Theory Study of Sulfur Poisoning", **J. Chem. Phys.**, 122 (2005) 84709

80. X.-Q. Gong, R. Raval and P. Hu: "CHx Hydrogenation on Co(0001): A Density Functional Theory Study", **J. Chem. Phys.**, 122 (2005) 24711

79. X.-Q. Gong, R. Raval and P. Hu: "General Insight into CO Oxidation: A Density Functional Theory Study of The Reaction Mechanism on Platinum Oxides", **Phys. Rev. Lett.**, 93 (2004) 106104-10607

78. X.-Q. Gong, R. Raval and P. Hu: "A Density Functional Theory Study on The Water Formation at High Coverages And The Water Effect in The Fischer-Tropsch Synthesis", **Molecular Physics**, 102 (2004) 993-1000

77. X.-Q. Gong, R. Raval and P. Hu: "CO dissociation and O removal on Co(0001): A Density Functional Theory Study", **Surf. Sci.**, 562 (2004) 247-256

76. R. Burch, S.T. Daniells and P. Hu: "The mechanism of N_2O formation via the $(NO)_2$ dimer: A density functional theory study**", J. Chem. Phys.**, 121 (2004) 2737-2745

75. R. Burch, S.T. Daniells, J.P. Breen and P. Hu: "A Combined Transient and Computational Study of the Dissociation of N_2O on Platinum Catalysts", **J. Catalysis**, 224 (2004) 252-260

74. R. Burch, S.T. Daniells, J.P. Breen and P. Hu: "The Effect of H_2 and the Presence of Hot-$O_{(ads)}$ During the Decomposition of N_2O on Platinum", **Catalysis Letters**, **94** (2004) 103

73. Z.-P. Liu and P. Hu: "CO Oxidation and NO Reduction on Metal Surfaces: Density Functional Theory Investigations", **Topics in Catalysis**, **28** (2004) 71-78

72. E.A. Armstrong, R.T. Brown, M.S. Sekwale, N.C. Fletcher, X.-Q. Gong and P. Hu: "The Unexpected Preference for the fac-Isomer with the Tris(5-seter-substitued-2,2'-bipyridine) Complexes of Ruthenium(II)", **Inorg. Chem.**, **43** (2004) 1714-1722

71. R.J. Mukerji, A.S. Bolina, W.A. Brown, Z.-P. Liu and P. Hu: "The Temperature Dependence of the Adsorption of NO on Pt(211): A RAIRS and DFT Investigation", **J. Phys. Chem.**, **108** (2004) 289-296

70. X.-Q. Gong, Z.-P. Liu, R. Raval and P. Hu: "A Systematic Study of CO Oxidation on Metals and Metal Oxides: Density Functional Theory Calculations", **J. Am. Chem. Soc.**, **126** (2004) 8

69. Z.-P. Liu, X.-Q. Gong, J. Kohanoff, C. Sanchez, P. Hu: "Catalytic Role of Metal Oxides in Gold-based Catalysts: A First Principles Study of CO Oxidation on TiO_2 Supported Au", **Phys. Rev. Lett.**, **91** (2003) 266102

68. Z.-P. Liu, P. Hu and M.-H. Lee: “Insight into Association Reactions on Metal Surfaces: Density Functional Theory Studies of Hydrogenation Reactions on Rh(111)”, **J. Chem. Phys.**, 119 (2003) 6282-6289

67. X.-Q. Gong, P. Hu and R. Raval: “The Catalytic Role of Water in CO Oxidation”, **J. Chem. Phys.**, 119 (2003) 6324-6334

66. A. Michaelides, P. Hu, M.-H. lee, A. Alavi and D.A. King: “Resolution of an Ancient Surface Science Anomaly: Work Function Change Induced by N Adsorption on W(100)”, **Phys. Rev. Lett.**, 90 (2003) 246103

65. A. Michaelides, Z.-P. Liu, C.J Zhang, A. Alavi, D. A. King and P. Hu: “Identification of General linear relationships between activation energies and enthalpy changes for reactions at surfaces”, **J. Am. Chem. Soc.**, 125 (2003) 3704-3705

64. Z.-P. Liu and P. Hu: “General Rules for Predicting Where a Catalytic Reaction Should Occur on Metal Surfaces: A Density Functional Theory Study of C-H and C-O Bond Breaking/Making on Flat, Stepped and Kinked Metal Surfaces”, **J. Am. Chem. Soc.**, 125 (2003) 1958-1967

63. R. Burch, G.A. Attard, S.T. Daniells, D.J. Jenkins, J.P. Breen and P. Hu: “Low Temperature Catalytic Decomposition of N_2O on Platinum and Bismuth-Modified Platinum: Identification of Active Sites”, **Chem. Commun.**, 22 (2002) 2738-2739

62. Z.-P. Liu, P. Hu and A. Alavi: “The Catalytic Role of Gold in Gold-Based Catalysts: A Density Functional Theory Study on the CO Oxidation on Gold”, **J. Am. Chem. Soc.**, 124 (2002) 14770-14779

61. Z.-P. Liu and P. Hu: “Mechanism of H_2 metabolism on Fe-only hydrogenases”, **J. Chem. Phys.**, 117 (2002) 8177-8180

60. Z.-P. Liu and P. Hu: “A New Insight into Fischer-Tropsch Synthesis”, **J. Am. Chem. Soc.**, 124 (2002) 11568-11569

59. R. Burch, S.T. Daniells and P. Hu: “N_2O and NO_2 Formation on Pt(111): A Density Functional Theory Study”, **J. Chem. Phys.**, 117 (2002) 2902-2908

58. Z.-P. Liu and P. Hu: “A Density Functional Theory Study on the Active Center of Fe-Only Hydrogenase: Characterization and Electronic Structure of the Redox States”, **J. Am. Chem. Soc.**, 124 (2002) 5175-5182

57. R.J. Baxter and P. Hu: “An Insight into Why the Langmuir-Hinshelwood Mechanism Is Generally Preferred”, **J. Chem. Phys.**, 116 (2002) 4379-4381

56. C.J. Zhang and P. Hu: “The Possibility of Single C-H Bond Activation in CH_4 on a MoO_3-Supported Pt Catalyst: A Density Functional Theory Study”, **J. Chem. Phys.**, 116 (2002) 4281-4285

55. C.J. Zhang, M. Lynch and P. Hu: "A Density Functional Theory Study of Stepwise Addition Reactions in Ammonia Synthesis on Ru(0001)", **Surf. Sci.**, 496 (2002) 221-230

54. C.J. Zhang and P. Hu: "Methane Transformation to Carbon and Hydrogen on Pd(100): Pathways and Energics from Density Functional Theory Calculations", **J. Chem. Phys.**, 116 (2002) 322-327

53. A. Michaelides and P. Hu: "Catalysis and Secret World of Atoms", **The Irish Scientist**, 9 (2001) 167-167

52. Z.-P. Liu and P. Hu: "An Insight into Alkali Promotion: A Density Functional Theory Study of CO Dissociation on K/Rh(111)", **J. Am. Chem. Soc.**, 123 (2001) 12596-12604

51. Z.-P. Liu and P. Hu: "General Trends in the Barriers of Catalytic Reactions on Transition Metal Surfaces", **J. Chem. Phys.**, 115 (2001) 4977-4980

50. C.J. Zhang and P. Hu: "A First Principles Study of Methanol Decomposition on Pd(111): Mechanisms for O-H Bond Scission and C-O Bond Scission", **J. Chem. Phys.**, 115 (2001) 7182-7186

49. A. Michaelides and P. Hu: "Hydrogenation of S to H_2S on Pt(111): A First-Principles Study", **J. Chem. Phys.**, 115 (2001) 8570-8574

48. C.J. Zhang, R.J. Baxter, P. Hu, A. Alavi and M.-H. Lee: "A Density Functional Theory Study of Carbon Monoxide Oxidation on the Cu3Pt(111) Alloy Surface: Comparison with the Reaction on Pt(111) and Cu(111)", **J. Chem. Phys.**, 115 (2001) 5272-5277

47. A. Michaelides and P. Hu: "The Valency Effect on Reaction Pathways in Heterogeneous Catalysis: Insight from Density Functional Theory Calculations", in *Theoretical Aspects of Heterogeneous Catalysis*, edited by M.A.C. Nascimento, published by Klewer (2001).

46. C.J. Zhang, Z.-P. Liu and P. Hu: "Stepwise Addition Reactions in Ammonia Synthesis: A First Principles Study", **J. Chem. Phys.**, 115 (2001) 609-611

45. Z.-P. Liu and P. Hu: "General Trends in CO Dissociation on Transition Metal Surfaces",**J. Chem. Phys.**, 114 (2001) 8244-8247

44. C.J. Zhang, P. Hu and A. Alavi: "Insight into Electron-Mediated Reaction Mechanisms: Catalytic CO Oxidation on a Ruthenium Surface", **J. Chem. Phys.**, 114 (2001) 8113-8118

43. A. Michaelides and P. Hu: "Catalytic Water Formation on Platinum: A First Principles Study", **J. Am. Chem. Soc.**, 123 (2001) 4235-4242

42. Z.-P. Liu, P. Hu and A. Alavi: “Mechanism for the High Reactivity of CO Oxidation on a Ruthenium-Oxide”, **J. Chem. Phys.**, 114 (2001) 5956-5957

41. A. Michaelides and P. Hu: “A Density Functional Theory Study of the Reaction of C+O, C+N and C+H on Close Packed Metal Surfaces”, **J. Chem. Phys.**, 114 (2001) 5792-5795

40. A. Michaelides and P. Hu: “Softened C-H Modes of Adsorbed Methyl and Their Implications for Dehydrogenation: an *Ab Initio* Study”, **J. Chem. Phys.**, 114 (2001) 2523-2526

39. C.J. Zhang and P. Hu: “CO Oxidation on Pd(100) and Pd(111): A Comparative Study of Reaction Pathways and Reactivity at Low and Medium Coverages”, **J. Am. Chem. Soc.**, 123 (2001) 1166-1172

38. A. Michaelides and P. Hu: “A Density Functional Theory Study of Hydroxyl and the Intermediate in the Water Formation Reaction on Pt”, **J. Chem. Phys.**, **114** (2001) 513-519

37. A. Michaelides and P. Hu: “Insight into Microscopic Reaction Pathways in Heterogeneous Catalysis”, **J. Am. Chem. Soc.**, **122** (2000) 9866-9867

36. N.D. McClenaghan, P. Hu and C. Hardacre: “A Density Functional Theory Study of the Surface Relaxation and Reactivity of Cu2O(100)”, **Surf. Sci.**, 464 (2000) 223-232

35. M. Lynch and P. Hu: “A Density Functional Theory Study of CO and Atomic Oxygen Chemisorption on Pt(111)”, **Surf. Sci.**, **458** (2000) 1-14

34. C.J. Zhang, P. Hu and A. Alavi: “A Density Functional Theory Study of CO Oxidation on Ru(0001) at Low Coverage”, **J. Chem. Phys.**, **112** (2000) 10564-10570

33. A. Michaelides and P. Hu: “A First Principles of CH_3 Dehydrogenation on Ni(111)”, **J. Chem. Phys.**, **112** (2000) 8120-8125

32. A. Michaelides and P. Hu: “A Density Functional Theory Study of CH_2 and H Adsorption on Ni(111)”, **J. Chem. Phys.**, **112** (2000) 6006-6014

31. C.J. Zhang and P. Hu: “Why Must Oxygen Atoms Be Activated from Hollow Sites to Bridge Sites in Catalytic CO Oxidation?”, **J. Am. Chem. Soc.**, **122** (2000) 2134-2135

30. C.J. Zhang, P. Hu and A. Alavi: “A General Mechanism for CO Oxidation on Close-packed Transition Metal Surfaces”, **J. Am. Chem. Soc.**, **121** (1999) 7931-7932

29. A. Michaelides and P. Hu: “Methyl Chemisorption on Ni(111) and C-H-M Multicentre Bonding: A Density Functional Theory Study”, **Surf. Sci.**, **437** (1999) 362-376

28. K. Bleakley and P. Hu: “A Density Functional Theory Study of the Interaction between CO and O on a Pt Surface: CO/Pt(111), O/Pt(111) and CO/O/Pt(111**)”, J. Am. Chem. Soc.**, **121** (1999) 7644-7652

27. A. Michaelides, P. Hu and A. Alavi: “Physical Origin of the High Reactivity of Subsurface Hydrogen in Catalytic Hydrogenation”, **J. Chem. Phys.**, **111** (1999) 1343-1345

26. C.J. Zhang, P. Hu and M.-H. Lee: “A Density Functional Theory Study on the Interaction between Chemisorbed CO and S on Rh(111)”, **Surf. Sci.**, **432** (1999) 305-315

25. J.J. Rooney and P. Hu: “A Comment on Mecho-catalytic Overall Water Splitting”, **Applied Catalysis A-General, 177** (1999) 9-9

24. A. Alavi, P. Hu, T. Deutsch, P.L. Silvestrelli and J. Hutter: “CO Oxidation on Pt(111): An Ab Initio Density Functional Theory Study”, **Phys. Rev. Lett., 80** (1998) 3650-3653

23. P. Hu, D.A. King, S. Crampin, M.-H. Lee and M.C. Payne: “Ab Initio Diffusional Potential Energy Surface CO chemisorption on Pd{110} at High Coverage: Coupled Translation and Rotation”, **J. Chem. Phys.**, **107** (1997) 8103-8109

22. Q. Ge, P. Hu, D.A. King, M.-H. Lee, J.A. White and M.C. Payne: “Site Symmetry Dependence of Repulsive Interactions between Chemisorbed Oxygen Atoms on Pt(111)-(1x1)”, **J. Chem. Phys., 106** (1997) 1210-1215

21. P. Hu, D.A. King, M.-H. Lee and M.C. Payne: “Orbital Mixing in CO Chemisorption on Transition Metal Surfaces”, **Chem. Phys. Letters**, **246** (1995) 73-78

20. P. Kaukasoina, M. Lindroos, P. Hu, D.A. King and C.J. Barnes: “Full Structure Determination of an Alkali Metal/CO co-Adsorption Phase, for Co{1010}-c(2x2)-(K+CO)”, **Phys. Rev. B**, **51** (1995) 17063-17067

19. M.P. Bessent, P. Hu, A. Wander and D.A. King: “A Novel Buckled Layer Structure for Atomic Adsorption on W{100}: the c(2x2)-Nitrogen Structure from Automated Tensor LEED”, **Surface Science**, **325** (1995) 272-278

18. P. Hu, D.A. King, S. Crampin, M.-H. Lee and C.M. Payne: “Gradient Corrections in Density Functional Theory Calculations for Surfaces: CO on Pd{110}”, **Chem. Phys. Letters**, **230** (1994) 501-506

17. L.D. Mapledoram, A. Wander, P. Hu and D.A. King: “Ambiguities in Adsorbate Site Assignment from Vibrational Frequencis Revealed by LEED”, in The Structure of Surfaces IV, edited by Xide Xie, S.Y. Tong and M.A. Van Hove, Proceedings of the 4th International Conference on the Structure of Surfaces (World Science, 1994)

16. A. Wander, P. Hu, M.P. Bessend and D.A. King: “Observation of a New Class of Reconstruction: An Adsorbate Stabilised Vacancy Structure for c(2x2)-X-W{100}”, in The Structure of Surfaces IV, edited by Xide Xie, S.Y. Tong and M.A. Van Hove, Proceedings of the 4th International Conference on the Structure of Surfaces (World Science, 1994)

15. P. Hu and D.A. King: “Cluster LEED: A Very Fast Method for Surface Structure Determinations”, **Phys. Rev. B**, **49** (1994) 2791-2800

14. P. Hu and D.A. King: “Comment on the ‘Blocking’ Model for Auger Emission Intensity Maps from Surface Structures”, **J. Phys. Chem.**, **97** (1993) 7379-7380

13. P. Hu, A. Wander, L.M. de la Garza, M.P. Bessent and D.A. King: “An Adsorbate-stabilised Vacancy Structure for Cu on W{100}: a Surface Alloy”, **Surface Science**, **286** (1993) L542-L546

12. P. Hu and D.A. King: “Viewing LEED Patterns as Electron Holograms”, Applied **Surface Science**, **70/71** (1993) 396-401

11. A. Wander, P. Hu and D.A. King: “Ambiguities in Adsorbate Site Assignment from Vibrational Frequencies: A TLEED Structural Study of (2x1) CO-Pd{110}”, **Chem. Phys. Letters**, **201** (1993) 393-398

10. P. Hu and D.A. King: “A Direct Inversion Method for Surface Structural Determination from LEED Intensities”, **Nature**, **360** (1992) 656-658

9. T. Masuda, C.J. Barnes, P. Hu and D.A. King: “Frendel-Kontorova Domain-Wall Phase Transitions in an Adsorbed Layer: Potassium on Co{1010}”, **Surface Science**, **275** (1992) 122-138

8. P. Hu and D.A. King: “Multiple Scattering Effects in Holographic Images”, **Phys. Rev. B**, **46** (1992) 13615-13618

7. P. Hu, C.J. Barnes and D.A. King: “Dominace of Short Range Order Effects in LEED Intensity Spectra”, **Phys. Rev. B**, **45** (1992) 13595-13598

6. P. Hu and D.A. King: “Holographic Images of Iodine Atoms on a Silver Surface from Electron Emission Patterns”, **Nature**, **353** (1991) 831-833

5. P. Hu, C.J. Barnes and D.A. King: “A Study on the Holographic Transform for Electron Diffraction from Surfaces”, **Chem. Phys. Letters**, **183** (1991) 521-528

4. C.J. Barnes, P. Hu, M. Lindroos and D.A. King: “The Surface Structure of a c(2x2) Potassium Overlayer on Co{1010}”, **Surface Science**, **251/252** (1991) 561-567

3. P. Hu, L.M. de la Garza, R. Raval and D.A. King: “A LEED Structural Study of the CO-induced Reconstruction of Pd{110}: Evidence for a Missing Row Structure”, **Surface Science**, **249** (1991) 1-7

2. M. Lindroos, C.J. Barnes, P. Hu and D.A. King: “The Termination and Multilayer Relaxation of the Co{1010} Surface”, **Chem. Phys. Letters**, **173** (1990) 92-96

1. P. Hu and Huang Deyin: “A Study of the Distribution of Latent Image in Core-Shell Emulsion Grains”, in: Progress in Basic Principles of Images Systems”, Proceedings of the International Congress of Photographic Science, Koln, Germany, 1986