Name	RAJEEV K. PATHAK
Qualification	M.Sc., Ph.D., Postdoc(USA)
Designation	Professor
Specialization	Theoretical Physics
Email	pathak@physics.unipune.ernet.in
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1 Education

	Course	Institution	Year
1	B.Sc. (Physics)	Fergusson College, University of Pune	1976
2	M.Sc. (Physics)	Department of Physics, University of Pune	1978
3	Ph.D. (theoretical Physics)	Department of Physics, University of Pune	1982

2 Career Profile

	Organisation / Institution	Designation	Duration
1	University of North Carolina, Chapel Hill, NC, USA	Postdoctora	
2	Tulane University, New Orleans, LA, USA	Postdictoral Fellow	1
3	University of Pune, Pune, India	Present: Professor	1989-to d
4	Tulane University, New Orleans, LA, USA	VISITING PROFESS	

3 Teaching Experience (Subjects/Courses Taught)

20 years' teaching experience. Quantum Mechanics-I, Quantum Mechanics-II, Quantum
Undergraduate level: Physics 122 (Algebra based) to 3 sections at Tulane, New Orleans

4 Research Interests / Specialization

Density Functional Theory, Electron Momentum Density, Mathematical Inequalities in P

5 Honors & Awards

UGC Career Award; Member, International Advisory Board for Electron Systems (Bosto

6 Publication - Books, Journals, Articles

	Year of Publication	Title	Co-Author
1	PLEASE SE BELOW: 51 Research Papers in International Journals.		
2			
3			

7 Publication - Conference Presentations New Orleans, LA, USA (2008); A

8 Professional Societies Memberships Member, The American Physical

9 Public Service / University Service / Consulting Activity

Have completed several research schemes: (i) UGC, New Delhi: Compton “Defect”; (ii) UGC Career Award Scheme (Atomic Energies, Positron-States, Density Functional Theory) (iii) C-DAC Project (iv) University-Potential-for-Excellence Award of a Research Scheme (on-going) for study of molecular nano-size clusters and their behavior in Electric Field

10 Projects (Major Grants / Collaborations)

11 Other Details

1. Direct and Reverse Transformations between Electron Density and Electron Momentum Density
* S. R. Gadre and R. K. Pathak
Physical Review – A (American Physical Society)

Volume A24, pages 2906-2912 (Year :1981).

2. Estimation of <p> and <1/p> from Atomic Electron Densities

*R. K. Pathak and S.R.Gadre

Journal of Chemical Physics (of the American Institute of Physics)

Volume 74, pages 5925-5926 (Year : 1981).

3. On Representation of the Coulomb Integral by One-Electron Functional

* S. R. Gadre and R. K. Pathak

Journal of Chemical Physics 75, 4740-4741 (1981).

4. Local Density Functional Model for Atoms in Momentum Space

*R. K. Pathak, P. V. Panat and S. R. Gadre

Physics Review – A25, 3073-3077 (1982).

5. Lower Bounds to the Weizsäcker Correction

* S. R. Gadre and R.K. Pathak

Physical Review – A25, 668-670 (1982).

6. Relationships between the Terms in the Gradient Expansion :Kinetic and Exchange Energy Functionals

* R. K. Pathak and S. R. Gadre

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7. Estimation of <p> and <1/p> from Atomic Electron Densities :

A. comment

* S. R. Gadre and R. K. Pathak

Journal of Chemical Physics 77, 1073-1073 (1983).

8. On Monotonicity of the Atomic Electron Momentum Density and The Shell-

Structure Characteristics of the Radial Momentum Density

* S. R. Gadre, S.J. Charavorty and R.K.Pathak

Journal of Chemical Physics, 78, 4581-4584 (1983).

9. Electron Density to Electron Momentum Density : The use of an Energy Constraint

* S. R. Gadre, S. P. Gejji and R. K. Pathak

Physical Review – A27, 3328-3331 (1983).

10. Electron Density to Electron Momentum Density: Connection with the Locally Averaged Method.
* S. R. Gadre, S. P. Gejji and R. K. Pathak
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11. Gradient-free Representation of the Weizsäcker term for Atoms.
* R. K. Pathak and S. R. Gadre
Physical Review – A28, 1808-1809 (1983).

12. An Upper Bound to the Exchange Integral for Coulomb Interactions
* R. K. Pathak
Journal of Chemical Physics 80, 583-584 (1984).

13. Bound Excited States within Density Functional Formalism: The Levy functional.
* R. K.Pathak
Physical Review – A29, 978-979 (1984).

14. From Molecular Electron Density to Electron Momentum Density
* R. K. Pathak, S. P. Gejji and S. R. Gadre

Physical Review – A29, 3402- 3405 (1984).

15. Statistical Electron Angular Correlation Coefficients within the Hohenberg - Kohn - Sham Theory, for Atomic Systems

* R. K. Pathak

Physical Review – A31, 2806-2809 (1985).

16. Relationships among the Terms in the Gradient Expansion of the Kinetic and Exchange-Correlation Energy Functionals. II

* R.K. Pathak and L.J. Bartolotti

Physical Review – A31, 3557-3564 (1985).

17. Approximate Relationships between Density Power Integrals, Moments of the Momentum Density and Interelectronic Repulsions in Diatomic Molecules

* R. K. Pathak, B. S. Sharma and A. J. Thakkar

Journal of Chemical Physics 85, 958-962 (1986).

18. Fourth- Order Gradient Expansion of the Fermion Kinetic Energy:

Extra Terms for Non-Analytic Densities

*J. P. Perdew, V. Sahni, M. Harbola and R.K. Pathak

Physical Review- B-34, 686-691 (1986).

19. Very Short –range Interatiomic Potentials

* R. K. Pathak and A. J. Thakkar

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20. Indirect-path Method for Atomic and Molecular Energies, and New Koopmans Theorems

* M. Levy, R. K. Pathak, J.P. Perdew and S.Wei

Physical Review- A36, 2491 –2494 (1987). (Rapid Communication)

21. Interconnections between Electron Densities in Position and Momentum spaces

* S. R. Gadre and R. K. Pathak

In Lecture Notes in Chemistry series, by Springer-Verlag, Vienna

Volume 50 (1988), (18 pages).

22. Bounds to Electron-Repulsion Integrals (Invited Article)

* S. R. Gadre and R. K. Pathak

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23. Developments of Links between Electron Densities in Complementary Spaces

* R. K. Pathak and S. R. Gadre

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24. Rigorous Bounds to Molecular Electron Repulsion and Electrostatic Potential Integrals

* S. R. Gadre, S.A. Kulkarni and R. K. Pathak

Journal of Chemical Physics, 91, 3596-3602 (1989).

25. Reduced First-order Density Matrices and "Exchange-only" Correlation-Factors for some Closed-shell Atomic Systems.

* S. R. Gadre, S.A. Kulkarni and R.K. Pathak

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*R. K. Pathak and P. V.Panat

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27. Atomic and Molecular Diamagnetic Susceptibilities from Compton Scattering Data

* S. R. Gadre and R.K. Pathak

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28. Momentum Space Atomic First-Order Density Matrices and "Exchange –only" Correlation Factors.

* R. K. Pathak, S. A. Kulkarni and S. R. Gadre

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29. Maximal and Minimal Characteristics of Molecular Electrostatic Potentials

* R. K. Pathak and S. R. Gadre

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30. Non-occurrence of Non-nuclear Strict Maxima in Molecular Electrostatic Potentials (Invited Article)

* S. R. Gadre and R.K. Pathak

Proceedings of the Indian Academy of Sciences, Vol.102,

pp.189-192 (1990).

31. Reply to the Comment on "Maximal and Minimal Characteristics of Molecular Electrostatic Potentials" : Some Further Extensions.

* S. R. Gadre, S. A. Kulkarni and R.K. Pathak

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32 . Bounds to Atomic and Molecular Energy Functionals

* S. R. Gadre and R. K. Pathak

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33. Topographical View of Molecular Electron Momentum Density

* S. A. Kulkarni, S. R. Gadre and R.K. Pathak
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* S. R. Gadre, S. A. Kulkarni and R. K. Pathak
Journal of Chemical Physics, 98, 3574-3576 (1993).

35. Leading Corrections to the Atomic Impulse-approximation Comption

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* R. K. Pathak, A. Kshirsagar, R. Hoffmeyer and A. J. Thakkar
Physical Review-A48, 2946-2951 (1993).

36. A necessary Condition for Atom-Positron Bound State
* R. K. Pathak
Physical Review-A50, 2191-2196 (1994).

37. Positron Binding: A Positron-Density Viewpoint
* T. Baruah, R.R. Zope, A. Kshirsagar and R. K. Pathak
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* R. R. Zope, M. K. Harbola and R. K. Pathak

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42. *Ab initio* Studies of anionic water pentamer clusters

* S. A. Kulkarni, L. J. Bartolotti and R. K. Pathak

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43. *Ab initio* investigations on neutral clusters of ammonia: $(NH_3)n$ (n=2-6)

* S. A. Kulkarni and R. K. Pathak

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44. *Ab initio* investigations on neutral Hydrogen Peroxide clusters: $(H_2O_2)_n$ (n=2,4)

* S. A. Kulkarni, L. J. Bartolotti and R. K. Pathak

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45. Structures, energetics and vibrational Spectra of $(H_2O_2)\cdots(H_2O_2)_n$ n = 1-6 : Ab Initio quantum chemical investigations

*A.D. Kulkarni, R.K. Pathak and L.J. Bartolotti

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*M.K. Harbola, R.R. Zope, A. Kshirsagar and R. K. Pathak

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* A.D. Kulkarni, R.K. Pathak and L.J. Bartolotti

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48. Interaction of peroxyformic acid with water molecules: A first-principles study

* A.D. Kulkarni, D. Rai, L.J. Bartolotti, and R.K. Pathak

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* D. Rai, H. Joshi, A.D. Kulkarni, S.P. Gejji, and R.K. Pathak

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50. The Methyl-hydroperoxide dimer: a Novel Molecular Cluster

* A.D. Kulkarni, D. Rai, L.J. Bartolotti and R.K. Pathak

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* D. Rai, A. D. Kulkarni, S. P. Gejji, and R. K. Pat

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Details
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Society; Fellow, Maharashtra Academy of Sciences

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