

Name	RAJEEV K. PATHAK
Qualification	M.Sc., Ph.D., Postdoc(USA)
Designation	Professor
Specialization	Theoretical Physics pathak@physics.unipune.ernet.in
Email	
Phone	92 202 569 9072, Ext 324

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	Postdoctoral Fellow	1982-1984
2	Tulane University, New Orleans, LA, USA	Postdoctoral Fellow	1984-1986
3	University of Pune, Pune, India	Present: Professor	1989-to date
4	Tulane University, New Orleans, LA, USA	VISITING PROFESSOR	1986-1988

3 Teaching Experience (Subjects/Courses Taught)

20 years' teaching experience. Quantum Mechanics-I, Quantum Mechanics-II, Quantum Field Theory, Statistical Physics, Solid State Physics, Condensed Matter Physics, Undergraduate level: Physics 122 (Algebra based) to 3 sections at Tulane, New Orleans; Graduate level: Physics 501, 502, 503, 504, 505, 506, 507, 508, 509, 510, 511, 512, 513, 514, 515, 516, 517, 518, 519, 520, 521, 522, 523, 524, 525, 526, 527, 528, 529, 530, 531, 532, 533, 534, 535, 536, 537, 538, 539, 540, 541, 542, 543, 544, 545, 546, 547, 548, 549, 550, 551, 552, 553, 554, 555, 556, 557, 558, 559, 5510, 5511, 5512, 5513, 5514, 5515, 5516, 5517, 5518, 5519, 5520, 5521, 5522, 5523, 5524, 5525, 5526, 5527, 5528, 5529, 5530, 5531, 5532, 5533, 5534, 5535, 5536, 5537, 5538, 5539, 5540, 5541, 5542, 5543, 5544, 5545, 5546, 5547, 5548, 5549, 5550, 5551, 5552, 5553, 5554, 5555, 5556, 5557, 5558, 5559, 5560, 5561, 5562, 5563, 5564, 5565, 5566, 5567, 5568, 5569, 5570, 5571, 5572, 5573, 5574, 5575, 5576, 5577, 5578, 5579, 5580, 5581, 5582, 5583, 5584, 5585, 5586, 5587, 5588, 5589, 5590, 5591, 5592, 5593, 5594, 5595, 5596, 5597, 5598, 5599, 55100, 55101, 55102, 55103, 55104, 55105, 55106, 55107, 55108, 55109, 55110, 55111, 55112, 55113, 55114, 55115, 55116, 55117, 55118, 55119, 55120, 55121, 55122, 55123, 55124, 55125, 55126, 55127, 55128, 55129, 55130, 55131, 55132, 55133, 55134, 55135, 55136, 55137, 55138, 55139, 55140, 55141, 55142, 55143, 55144, 55145, 55146, 55147, 55148, 55149, 55150, 55151, 55152, 55153, 55154, 55155, 55156, 55157, 55158, 55159, 55160, 55161, 55162, 55163, 55164, 55165, 55166, 55167, 55168, 55169, 55170, 55171, 55172, 55173, 55174, 55175, 55176, 55177, 55178, 55179, 55180, 55181, 55182, 55183, 55184, 55185, 55186, 55187, 55188, 55189, 55190, 55191, 55192, 55193, 55194, 55195, 55196, 55197, 55198, 55199, 551000, 551001, 551002, 551003, 551004, 551005, 551006, 551007, 551008, 551009, 5510010, 5510011, 5510012, 5510013, 5510014, 5510015, 5510016, 5510017, 5510018, 5510019, 55100100, 55100101, 55100102, 55100103, 55100104, 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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 $\langle p \rangle$
and $\langle 1/p \rangle$ 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

Physical Review –
A25, 3426-3428 (1982).

7. Estimation of $\langle p \rangle$ and
 $\langle 1/p \rangle$ 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
Physical Review –
A28, 462-463 (1983).

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
Interatomic Potentials

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

Journal of Chemical
Physics 87, 2186 -2190
(1987).

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

Proceedings of The
Academy of Sciences-I
Vol.100, pp483-508
(1988).

23. Developments of
Links between Electron
Densities in

Complementary
Spaces

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

Portugalea Fisica
Vol.19, pp 407-408
(1988).

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
Physical Review –
B41, 4749-4751 (1989).

26. Critical Indices for
High – Tc Superconductors
*R. K. Pathak and P.
V.Panat
Physical Review- B41,
4749-4751 (1990).

27. Atomic and Molecular
Diamagnetic
Susceptibilities from
Compton
Scattering Data
* S. R. Gadre and R.K.
Pathak
Physical Review-A92.
4327-4330 (1990).

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

* R. K. Pathak, S. A.
Kulkarni and S. R. Gadre
Physical Review –
A42, 2622-2626 (1990).

29. Maximal and
Minimal Characteristics of
Molecular Electrostatic
Potentials
* R. K. Pathak and
S. R. Gadre
Journal of Chemical
Physics, 93, 1770-1773
(1990).

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
Journal of Chemical
Physics, 94, 8639-8639
(1991).

32 . Bounds to Atomic
and Molecular Energy
Functionals

* S. R. Gadre and R.
K. Pathak
Advances in
Quantum Chemistry,
Vol.22, pp.211-300
(Academic Press,
U.S.A., 1991).

33. Topographical View
of Molecular Electron
Momentum Density

* S. A. Kulkarni, S.
R. Gadre and R.K. Pathak
Physical Review-
A42, 4399-4406 (1992).

34. Density-based
Molecular Electron
Localization Functions

* 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 Compton

Profiles: A Density
Functional Approach
* 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
Physical Review-
A50, 2191-2196 (1994).

38. Leading Corrections
to Atomic Impulse
Approximation Compton
profiles: Second
order Correction
* R. R. Zope, A.
Kshirsagar and R. K.
Pathak
Chemical Physics
Letters (Elsevier,
Amsterdam)
Volume – 242, pp
555-559 (1995).

39. Indirect path
method: Accurate total
atomic energies

* M. K. Harbola, R.
R. Zope and R. K. Pathak
Physical Review –
A53, 3652-3656 (1996).

40. Density-Functional
approach to positron-
neutral atom bound states
* T. Baruah, R. K. Pathak,
A. Kshirsagar
Physical Review A55,
1518-1521 (1997).

41. Atomic Compton
Profiles Within different
“exchange-only” theories

* R. R. Zope, M. K.
Harbola and R. K. Pathak
European Physical
Journal D7, 151-155
(1999).

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

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

Journal of Chemical Physics 113, 2697-2700 (2000).

43. *Ab initio* investigations on neutral clusters of ammonia: $(\text{NH}_3)_n$ ($n=2-6$)

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

Chemical Physics Letters 336, 278-283 (2001).

44. *Ab initio* investigations on neutral Hydrogen Peroxide clusters: $(\text{H}_2\text{O}_2)_n$ ($n=2,4$)

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

Chemical Physics Letters 372, 620-626 (2003).

45. Structures, energetics and vibrational Spectra of $(\text{H}_2\text{O}_2)_{...}(\text{H}_2\text{O}_2)_n$ $n = 1-6$:

Ab Initio quantum chemical investigations

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

Journal of Physical
Chemistry (American
Chemical Society)
109, 4583-4590
(2005).

46. Momentum-space
properties from Co-
ordinate-space electron
density

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

Journal of Chemical
Physics 122, 204110 (1-5)
(2005).

47. Effect of additional
water on hydrated
hydrogen peroxide: a
quantum chemical study

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

Journal of Chemical
Physics 124, 214309(1-7)
(2006).

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

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

Journal of Physical
Chemistry -A 110 (42)
11855 -11861 (2006).

49. Electric field effects
on aromatic and aliphatic
hydrocarbons: A Density-
Functional study
* D. Rai, H. Joshi,
A.D. Kulkarni, S.P. Gejji,
and R.K. Pathak

Journal of Physical
Chemistry-A: 111 (37),
9111 -9121, 2007).

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

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

Journal of
Molecular Physics
THEOCHEM 824, 32-38
(2007).

51. Water clusters (H_2O)_n, n= 6-8 in external electric fi

* D. Rai, A. D. Kulkarni, S. P. Gejji, and R. K. Pat
Journal of Chemical Physics 128, 034310, (2008).

Details
86.20%, Stood First in Physics
18.30%, Stood First in Physics

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1 Mechanics-III, Quantum Mechanics-IV, Electrodynamics-I, Electroynam Classical Mechanics
s, LA, USA.

hysics, Molecular Clusters Clusters in External electric fields

n University), International Center for Theoretical Physics: Senior Group Associateship.

Book/Journal/Article

tlanta, GA, USA (2006); Boston, MA, USA (1997)

Society; Fellow, Maharashtra Academy of Sciences

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