

# **Curriculum Vitae**

**Hendrik J. Monkhorst**  
**Quantum Theory project**  
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Born: 13 October, 1938, Kampen, the Netherlands

## **Education**

PhD, Theoretical Chemistry, University of Groningen, 1968, the Netherlands

## **Professional Record**

- September 2000–June 2001, sabbatical, University of California, Irvine, Physics and Astronomy Department, and TriAlpha Energy, Inc
- 1983-present, Professor of Physics and Chemistry, University of Florida, Gainesville, Florida.
- 1982–1983, Associate Director of the Quantum Theory Project.
- 1982–1983, Associate Professor of Physics and Chemistry, University of Florida, Gainesville, Florida.
- 1978–1982, Associate Professor, Department of Physics, University of Florida, Gainesville, Florida.
- 1975–1978, Associate Research Professor, Physics Department, University of Utah, Salt Lake City, Utah.
- Summer 1974, Visiting Professor, Aarhus University, Aarhus, Denmark.
- 1973–1975, Assistant Research Professor, Physics Department, University of Utah, Salt Lake City, Utah.
- 1972–1973, Senior Research Associate, Physics Department, University of Utah, Salt Lake City, Utah.

- 1971–1972, Research Fellow, Institute “Rudjer Boskovic,” Zagreb, Croatia, Yugoslavia.
- 1968–1971, Research Associate and Associate Instructor, Physics Department, University of Utah, Salt Lake City, Utah.
- 1965–1968, Research Assistant, University of Groningen, The Netherlands.

## Awards and Honors

1. Hercules Powder Company Award for Outstanding Research in Physics, 1970
2. Fellow, American Physical Society, 1991
3. March 2003: Passed 2,000 citations mark of paper Special Points for Brillouin Zone Integrations, By H. J. Monkhorst and J. D. Pack, Phys.Rev B13, 5188(1976)
4. June 2005: Above article cited in Physics Today article “Citation Statistics from 110 Years of *Physical Review*: positions 11 and 6 on lists articles with “More than 1,000 citations” and “Hot Papers”, respectively

## Publications

1. “SCMO Calculations on the Tetramethyl p-phenylene Diamine System,” H.J. Monkhorst and J. Kommandeur, *J. Chem. Phys.* **47**, 391 (1967).
2. “Magnetic Transition of Wurster’s Blue Perchlorate. II. Theoretical Considerations,” H.J. Monkhorst, G.T. Pott and J. Kommandeur, *J. Chem. Phys.* **47**, 401 (1967).
3. “Activation Energy for Interconversion of Enantiomers Containing an Asymmetric Carbon Atom without Breaking Bonds,” H.J. Monkhorst, *Chem. Commun.* (1968), 1111.
4. “Inner-Shell/Outer-Shell Interaction in Approximate LCAO-SCF Calculations,” H.J. Monkhorst, Thesis, University of Groningen (1968).
5. “Geometrical Changes During the Internal Rotation in Ethane,” H.J. Monkhorst, *Chem. Phys. Letters* **3**, 289 (1969).
6. “Comments on ‘Geometrical Changes During the Internal Rotation in Ethane,’ ” H.J. Monkhorst, *Chem. Phys. Letters* **4**, 119 (1969).
7. “Multicenter Integrals via Gaussian Expansion of Slater-Orbital Products,” H.J. Monkhorst and F.E. Harris, *Chem. Phys. Letters* **3**, 537 (1969).
8. “Lattice Sums and Madelung Constants,” F.E. Harris and H.J. Monkhorst, *Chem. Phys. Letters* **4**, 181 (1969).

9. "Complete Calculations of the Electronic Energies of Solids," F.E. Harris and H.J. Monkhorst, Phys. Rev. Letters **23**, 1026 (1969).
10. "Application of New Madelung Summation Method to Close-Packed Alkali-Halide Structures," F.E. Harris and H.J. Monkhorst, J. Chem. Phys. **52**, 4310 (1970).
11. "Electronic-Structure Studies of Solids. I. Fourier Representation Method for Madelung Sums," F.E. Harris and H.J. Monkhorst, Phys. Rev. **B2**, 4400 (1970).
12. "Toward Hartree-Fock Calculations for Simple Crystals," F.E. Harris and H.J. Monkhorst, Computational Methods in Band Theory, P.M. Marcus, J.F. Janak and A.R. Williams, Eds. (Plenum Press, New York, 1971), pp. 517–541.
13. "'Exact' Hartree-Fock Calculations for Atomic-Hydrogen Crystal," F.E. Harris and H.J. Monkhorst, Solid State Comm. **9**, 1449 (1971).
14. "'Exact' Hartree-Fock Results for Atomic-Hydrogen Crystals," F.E. Harris, L. Kumar and H.J. Monkhorst, Int. J. Quantum Chm. **5**, 527 (1971).
15. "Accurate Calculation of Fourier Transform of Two-Center Slater Orbital Products," H.J. Monkhorst and F.E. Harris, Int. J. Quantum Chem. **6**, 601 (1972).
16. "The Exact Hartree-Fock Problem for Lithium Crystals: A Preliminary Report," F.E. Harris, L. Kumar and H.J. Monkhorst, J. de Physique **33** (C3), 99 (1972).
17. "On Localized Orbitals in Infinite, Periodic Systems," H.J. Monkhorst, Chem. Phys. Letters **17**, 461 (1972).
18. "Electronic-Structure Studies of Solids. II. 'Exact' Hartree-Fock Calculations for Cubic Atomic-Hydrogen Crystals," F.E. Harris, L. Kumar and H.J. Monkhorst, Phys. Rev. **B7**, 2850 (1973).
19. "Slater Orbital Molecular Integrals with Numerical Fourier Transform Methods. I. (Coplanar) Multicenter Exchange Integrals over 1s Orbitals," A Graovac, H.J. Monkhorst and T. Zivkovic, Int. J. Quantum Chem. **7**, 233 (1973).
20. "Random-Phase-Approximation Correlation Energy in Metallic Hydrogen Using Hartree-Fock Bloch Functions," H.J. Monkhorst and J. Oddershede, Phys. Rev. Letters **30**, 797 (1973).
21. "Electronic-Structure Studies of Solids. III. Hartree-Fock Band Functions and Energies for Cubic Lithium Crystals," L. Kumar, H.J. Monkhorst and F.E. Harris, Phys. Rev. **B9**, 4084 (1974).
22. "Electronic-Structure Studies of Solids. IV. Physical Quantities from Rigorous Hartree-Fock Results for Lithium Crystals," L. Kumar and H.J. Monkhorst, J. Phys. **F4**, 1135 (1974).
23. "On the Hartree-Fock Limit for Metallic Hydrogen with a Plane Wave Basis," J. Oddershede, L. Kumar and H.J. Monkhorst, Int. J. Quantum Chem. **S8**, 447 (1974).

24. "Computation of Fourier Transform Quantities in Hartree-Fock Calculations for Simple Crystals," A. Graovac, H.J. Monkhorst and M.L. Glasser, *Int. J. Quantum Chem.* **9**, 243 (1975).
25. "Comments on 'Self-Consistent Pair Correlation Approach to Many-Body Effects in Metals,'" H.J. Monkhorst, *Phys. Rev. B* **12**, 792 (1975).
26. "Note on Computation of the Fourier Transforms of Lattice Sums over Slater-Type Orbital Products," H.J. Monkhorst and A. Graovac, *Ann. Soc. Sci. Bruxelles* **89**, 252 (1975).
27. "Exact LCAO Method for Two-Dimensional Crystals Using Fourier Transform Techniques," H.J. Monkhorst.
28. "On Special Points for Brillouin Zone Integrations," H.J. Monkhorst and J.D. Pack, *Phys. Rev. B* **13**, 5188 (1976).
29. "Electronic-Structure Studies of Solids. V. Rigorous Hartree-Fock Treatment of Metallic Hydrogen Using a Plane-Wave Basis," L. Kumar, H. J. Monkhorst and J. Oddershede, *Int. J. Quantum Chem.* **12**, 145 (1977).
30. "Calculation of Properties with the Coupled-Cluster Method," H.J. Monkhorst, *Int. J. Quantum Chem.* **S11**, 421 (1977).
31. "Special Points for Brillouin-Zone Integrations—A Reply," J.D. Pack and H.J. Monkhorst, *Phys. Rev. B* **16**, 1748 (1977).
32. "Analytic Connection between Configuration-Interaction and Coupled-Cluster Methods," T.P. Zivkovic and H.J. Monkhorst, *J. Math. Phys.* **19**, 1007 (1978).
33. "On the X-Ray Scattering Factors of Metallic and Molecular Hydrogen Crystals," H.J. Monkhorst, J.D. Pack and D.L. Freeman, *Solid State Comm.* **29**, 735 (1979).
34. "Lithium Crystal Properties from High-Quality Hartree-Fock Wave Functions," J.D. Pack, H.J. Monkhorst and D.L. Freeman, *Solid State Comm.* **29**, 723 (1979).
35. "The High-Temperature Resistivity of Beryllium," H.J. Monkhorst and J.D. Pack, *Solid State Comm.* **29**, 625 (1979).
36. "Hartree -Fock Density-of-States for Extended Systems," H.J. Monkhorst, *Phys. Rev. B* **20**, 1504 (1979).
37. "No Linear Dependence and Multi-Center Integral Problems in Momentum Space Quantum Chemistry," H.J. Monkhorst and B. Jeziorski, *J. Chem. Phys.* **71**, 5268 (1979).
38. "Hartree-Fock Formalism for the Calculation of Total Energies and Charge Densities of Thin Films," F.E. Harris, H.J. Monkhorst and W.A. Schwalm, *J. Vac. Sci. Technology* **16**, 1318 (1979).

39. "The Contraction Theorem for the Algebraic Reduction of (Anti) Commutators Involving Operator Strings," F.E. Harris, B. Jeziorski and H.J. Monkhorst, Phys. Rev. **A23**, 1632 (1981).
40. "Recursive Scheme for Order-by-Order Many-Body Perturbation Theory," H.J. Monkhorst, B. Jeziorski and F.E. Harris, Phys. Rev. **A23**, 1639 (1981).
41. "Electrostatics for Periodic Films of Atoms," H.J. Monkhorst and W.A. Schwalm, Phys. Rev. **B23**, 1729 (1981).
42. "Coupled-Cluster Method for Multi-Determinantal Reference Space," B. Jeziorski and H.J. Monkhorst, Phys. Rev. **A24**, 1668 (1981).
43. "Exact Exchange Asymptotics in Polymer Hartree-Fock Calculations," H.J. Monkhorst and M. Kertesz, Phys. Rev. **B24**, 3015 (1981).
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72. "Molecular Effects in Tritium  $\beta$  Decay. III. Electronic Resonances of  $\text{HeT}^+$  Ion and the Dependence of the Neutrino Mass on Accuracy of the Theoretical Model," K. Szalewicz, O. Fackler, B. Jeziorski, W. Kolos and H.J. Monkhorst, Phys. Rev. A **35**, 965 (1987).
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## **Patents, Filed or Issued**

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