

Resume
Douglas J. Klein

Education:

B.Sc. at Oregon State University
M.Sc. & Ph.D. at University of Texas @ Austin

Professional:

Post-doc, Princeton University, chemistry
Assistant Professor, physics, University of Texas
Post-doc & visiting Assist. Prof., chemistry, Rice University
Scientific Officer (in physics), Office of Naval Research, Washington, D. C.
Assistant, Associate, & Full Professor, MARS, Texas A&M University @ Galveston

Fellowships, Awards, & Grants:

summer research assistantships, Los Alamos Natl. Labs
NAS/AFOSR fellowship at Princeton University
DAAD fellowship to Universitat zu Koln
~30 years of Welch Foundation Grants, for chemical research
Texas A&M University Research Award, 1992
PRF-ACS Grant, for chemical research
Fulbright Fellowship, Oxford University, 1994
Welch Foundation featured researcher 1997
dedicated "Klein Festschrift" in *Croatia Chemica Acta*, 2013
dedicated meeting "Conjugated-Carbon Nano-Structures" in Cuernavaca, Mexico, 2014
Regent's Professor TAMUG, 2016

Teaching, Lectures, etc:

- * Courses, in undergraduate physics, chemistry, & eco-environmental modelling, & "conjugated-carbon nano-structures" at TAMUG.
- * Special sets of notes, for MARS 470 Eco-environmental Modelling, as well as "Conjugated-Carbon Nano-Structures" special topics course, and also, abbreviated notes for PHYS 218 & for CHEM 107
- * A few undergrad physics & graduate chemistry courses sometime back at UT-Austin & Rice U.
- * Over 100 invited lectures (chemistry, physics, & math) in USA, Japan, Germany, Croatia, Spain, Slovenia, England, Canada, Mexico, China, & Columbia.
- * research with ~30 post-docs, ~4 grad students, and numerous visitors & collaborators
- * >400 professional publications; co-editorship for 2 books & for 3 special issues of journals.

Service

Numerous MARS & TAMUG committees over the last 4 decades
Editorship on ~5 journal editorial boards (currently 3)
Co-organizer for a couple scientific meetings

Some important Publications:

- * F. A. Matsen & D. J. Klein, "Spin Conservation", *Advances Photochem.*, **1969**, VII, 1-55 (ed. W. A. Noyes, Jr., G. S. Hammond, & J. N. Pitts; pub. John Wiley & Sons, NY).
- * D. J. Klein, "Local Permutational Symmetry and the Separated Atom Limit", *J. Chem. Phys.* **1969**, 50, 5140-5150.
- * D. J. Klein, C. H. Carlisle, & F. A. Matsen, "Symmetry Adaptation to Sequences of Finite Groups", *Adv. Quantum Chem.*, **1970**, 5, 219-260 (ed. P.O. Lowdin; Academic Press).

- * D. J. Klein, "Variational Scheme for Multistate Kets", *Phys. Rev. A* **1971**, *3*, 528-532.
- * D. J. Klein & W. A. Seitz, "Partially Filled Linear Hubbard Model Near the Atomic Limit", *Phys. Rev. B* **1974**, *10*, 3217-3226.
- * D. J. Klein & A. H. Cowley, "Permutational Isomerism", *J. Am. Chem. Soc.* **1975**, *97*, 1633-1640.
- * D. J. Klein & H. M. Pickett, "Nodal Hypersurfaces and Anderson's Random-Walk Simulation of the Schroedinger Equation", *J. Chem. Phys.* **1976**, *64*, 4811-4812
- * D. J. Klein & M. A. Garcia-Bach, "Variational Localized-Site Cluster Expansions. Dimerization in Linear Chains", *Phys. Rev. B* **1979**, *19*, 877-886.
- * W. Hasselbarth, E. Ruch, D. J. Klein, & T. H. Seligman, "Bilateral Classes", *J. Math. Phys.* **1980**, *21*, 951-953.
- * W. A. Seitz & D. J. Klein, "Monte Carlo Results for a Branched Polymer Model Including Volume Exclusion", *J. Chem. Phys.* **1981**, *77*, 5190-5193.
- * D. J. Klein, "Treedagonal Matrices & Their Inverses", *Linear Alg. & Its Appl.* **1982**, *42*, 109-117.
- * D. J. Klein, "Valence-Bond Theory for Conjugated Hydrocarbons", *Pure & Appl. Chem.* **1982**, *55*, 299-306.
- * R. D. Poshusta & D. J. Klein, "Novel *Ab Initio* Correlated Calculations for the Infinite Chain of Hydrogen Atoms", *Phys. Rev. Lett.* **1982**, *48*, 1555-1558.
- * D. J. Klein, "Semiregular Induction of Group Representations", *J. Math. Phys.* **1984**, *25*, 200-203.
- * D. J. Klein, T. G. Schmalz, G. E. Hite, & W. A. Seitz, "Resonance in C₆₀ Buckminsterfullerene", *J. Am. Chem. Soc.* **1986**, *108*, 1301-1302.
- * T. G. Schmalz, W. A. Seitz, D. J. Klein, & G. E. Hite, "Elemental Carbon Cages", *J. Am. Chem. Soc.* **1988**, *110*, 1113-1127.
- * D. J. Klein & N. Trinajstić, "Foundations of conjugated-circuits models", *Pure & Appl. Chem.* **1989**, *61*, 2107-2115.
- * D. J. Klein, T. P. Živković, & R. Valenti, "Topological Long-range Order for Resonating Valence-Bond Structures", *Phys. Rev. B* **1991**, *43*, 723-727.
- * D. J. Klein, "Aromaticity *via* Kekulé Structures & Conjugated Circuits", *J. Chem. Ed.* **1992**, *69*, 691-694.
- * D. J. Klein & X. Liu, "Theorems for Carbon Cages", *J. Math. Chem.* **1992**, *11*, 199-205.
- * D. J. Klein, W. A. Seitz, & T. G. Schmalz, "Symmetry of Infinite Tubular Polymers: Application to Buckytubes", *J. Phys. Chem.* **1993**, *97*, 1231-1236.
- * D. J. Klein & M. Randić, "Resistance Distance", *J. Math. Chem.* **1993**, *12*, 81-95.
- * H-Y. Zhu, D. J. Klein, W. A. Seitz, & N. H. March, "BN-Alternants: Boron Nitride Cages and Polymers", *Inorg. Chem.* **1995**, *34*, 1377-1383.
- * D. J. Klein, "Similarity and Dissimilarity in Posets", *J. Math. Chem.* **1995**, *18*, 321-348.
- * A. T. Balaban, D. Babić, & D. J. Klein, "W. R. Hamilton", *J. Chem. Ed.* **1995**, *72*, 693-698.
- * D.J. Klein & L. Bytautas; "Graphitic Edges & Unpaired π -Electron Spins", *J. Phys. Chem. A*, **1999**, *103*, 5196-5210.
- * L. Bytautas, D. J. Klein, T.G. Schmalz, "All acyclic hydrocarbons: formula periodic table & property overlap plots *via* chemical combinatorics", *New J. Chem.* **2000**, *24*, 329-336.
- * D. Babić, D.J. Klein, & T.G. Schmalz; "Curvature matching & strain relief in bucky-tori: usage of sp³-hybridization & nonhexagonal rings", *J. Mol. Graphics & Modelling*, **2001**, *19*, 223-231.

- * D. J. Klein; "Topo-combinatoric categorization of quasi-local graphitic defects", *Phys. Chem. – Chem. Phys.* **2002**, *4*, 2099-2110.
- * D. J. Klein & O. Ivanciuc, "Graph Cyclicity, Excess Conductance, & Resistance Deficit", *J. Math. Chem.* **2002**, *30*, 271-287.
- * T. Doslic & D. J. Klein, "Splinoïd interpolation on finite posets", *J. Comp. & Appl. Math.*, **2005**, *177*, 175-185.
- * T. Ivanciuc, D. J. Klein, & O. Ivanciuc, "Posetic Cluster Expansion for Substitution-Reaction Networks & Application to Methylated Cyclobutanes", *J. Math. Chem.* **2007**, *41*, 355-379.
- * D. J. Klein, "Defected/decorated benzenoid/graphitic nano-structures", *Pure & Appl. Chem.*, **2008**, *80*, 1399-1414.
- * A. Misra, T. G. Schmalz, & D. J. Klein, "Clar Theory for Radicaloid Benzenoids", *J. Chem. Info. & Modelling*, **2009**, *49*, 2670-2676.
- * D. J. Klein, "Centrality Measure in Graphs", *J. Math. Chem.* **2010**, *47*, 1209-1223.
- * G. Restrepo, R. Brüggemann, & D. J. Klein, "Partially Ordered Sets: Ranking & Prediction of Substances' Properties", *Current Computer-Aided Drug Design* **2011**, *7*, 133-145.
- * D. J. Klein & A. T. Balaban, "Clarology for Conjugated Carbon Nano-Structures: Molecules, Polymers, Graphene, Defected Graphene, Fractal Benzenoids, Fullerenes, Nano-Tubes, Nano-Cones, Nano-Tori, etc.", *Open J. Organic Chem.* **2011**, *5*, 27-61 (Suppl 1-M3).
- * D. J. Klein, "Spin-Free Quantum Electronic Structure: Its Second Quantization and Para-Fermionics", *Intl. J. Quantum Chem.* **2011**, *111*, 76-95.
- * Y. Yang & D. J. Klein, "Recursion Relations for Resistance Distance & Its Application", *Disc. Appl. Math.* **2013**, *161*, 2702-2715.
- * A. Panda, S. Vijayakumar, D. J. Klein, & A. Ryzhov, "Network of Secondary-Substituted Adamantane Amines", *J. Phys. Org. Chem.* **2013**, *26*, 917-926.
- * D. J. Klein, Y. Yang, & D. Ye, "HOMO-LUMO gaps for sub-graphenic & sub-buckytubic species", *Proc. Royal Soc. London A* **2015**, *471*, 20150183.
- * D. Bhattacharya, Y. Ortiz, & D. J. Klein, "The Astounding Buckyball-Buckyball", *Chem. Phys. Lett.* **2016**, *647*, 185-188.
- * T. Goswami, A. Panda, & D. J. Klein, "Spin-Density Localization in Graphene at Boundaries & at Vacancy Defects", *J. Phys. Chem. C* **2019**, *123*, 9479-9485.
- * J. M. Oliva-Enrich & D. J. Klein, "On the effect of charge & spin in $\text{He}^{(q)}@X_n Z_{12-n} H_{12}^{(n-2)}$ molecules, with $X = \{C, Si\}$, $Z = \{B, Al\}$ and $q = \{0, +1, +2\}$, $n = \{0, 1\}$ ". *Theor. Chem. Acc.* **2019**, *138*, 102:1-8.
- * D. J. Klein, T. Goswami, Y. Ortiz, "Translationally Symmetric Graphene Strips", *J. Math. Chem.* **2020**, (accepted).