

Good Afternoon, All:

Please accept this nomination of Dr. Douglas Klein for the ecological modeling vacancy on the EAHCP Science Committee. Dr. Klein's CV is ATTACHED, his statement of "no affiliation" with the EAHCP's contracted ecological modeling team is below, and his statement of willingness to serve is also included below, along with my original e-mail outreach to him.

Thank you,  
-Steve B.

**From:** Douglas Klein [mailto:kleind@tamug.edu]  
**Sent:** Thursday, July 17, 2014 2:14 PM  
**To:** Steven Bereyso  
**Subject:** FW: Invitation to Consider Joining the EAHCP Science Committee

Steven Bereyso

You asked whether I have any affiliation with any of these people:

Dr. Timothy Bonner	Texas State University (TSU) – Department of Biology
Dr. Gary Dick Dr. Tim Lewis Dr. Todd Swannack	USACE Engineering Research and Development Center (ERDC)
Dr. Robert Doyle	Baylor University – Center for Reservoirs and Aquatic Systems Research
Dr. Bill Grant Dr. Hsiaohsuan Wang	Texas A&M University (TAMU)– Department of Wildlife and Fisheries Sciences
Dr. Thomas Hardy	Watershed Systems Group, Inc. (WSG)
Mr. Ed Oborny	BIO-WEST, Inc.
Dr. George Ward	University of Texas – Center for Research in Water Resources (CRWR)

The answer is no. Except that in common with Drs Grant and Wang, we all work for the same university TAMU, albeit in different locations, and different departments.

Doug Klein

## RESUME: DOUGLAS J. KLEIN

BS in chemistry, Oregon State University 1964  
MS in chemistry & PhD in chemical physics, University of Texas (at Austin) 1967 & 1969  
post-doc, Princeton University 1970-71  
Asst. Prof. Physics, University of Texas (at Austin) 1971-1977  
post-doc & visiting Asst. Prof. Chemistry, Rice University, 1978-1979  
Asst., Assoc., & Full Prof. Texas A&M University @ Galveston 1979-2013  
Scientific Officer, Office of Naval Research 1984  
Fulbright fellow, Oxford University 1994

### Teaching at TAMUG

\* Introductory Chemistry

2-semester course for scientists

1-semester course for engineers

\* Introductory Physics

2-semester course (with calculus)

2-semester course (w/o calculus)

\* Eco-environmental Modelling

\* Conjugated-Carbon Nano-Structures

\* Marine Sciences Seminar

(some other courses earlier at Rice & UT-Austin: introductory physics, undergrad quantum mech., upper-div. classical mechanics, quantum chemistry, statistical thermodynamics)

### Research:

Collaboration with dozens of leading researchers, from around the world.

Numerous post-doctoral students at TAMUG, from a long-running Welch grant.

Research: electronic structure of molecular crystals, many-body theory, chemical (& mathematical) graph theory, polymer statistics, applications of group theory, semi-empirical resonating valence-bond theory, chemical enumerations, molecular magnetism, conjugated-carbon nano-structures

Over 300 research articles, two co-edited books, & 3 guest-edited special journal issues.

### Selected Publications

1. F. A. Matsen & D. J. Klein, "Spin Conservation", pages 1-55 in Advances in Photochemistry, Vol. VII, ed. by W. A. Noyes, Jr., G. S. Hammond and J. N. Pitts, Jr., (John Wiley and Sons, 1969).
2. D. J. Klein & Z. G. Soos, "Site Representation for Charge Transfer Excitations in Molecular Crystals", Molecular Physics 20 (1971) 1013-1024.
3. D. J. Klein & A. H. Cowley, "Permutational Isomerism", Journal of the American Chemical Society, 97 (1975) 1633-1640.
4. D. J. Klein & M. A. Garcia-Bach, "Variational Localized-Site Cluster Expansions. X. Dimerization in Linear Chains", Physical Review B 19 (1979) 877-886.
5. D. J. Klein & W. A. Seitz, "Graphs, Polymer Models, Excluded Volume, and Chemical Reality", pages 430-445 in Chemical Applications of Topology and Graph Theory, ed. R. B. King (Elsevier, Amsterdam, 1983).
6. D. J. Klein, "Valence-Bond Theory for Conjugated Hydrocarbons", Pure & Applied Chemistry 55 (1982) 299-306.
7. D. J. Klein, "Treedagonal Matrices and Their Inverses", Linear Algebra and Its Applications 42 (1982) 109-117.

8. D. J. Klein, T. G. Schmalz, G. E. Hite, & W. A. Seitz, "Resonance in C<sub>60</sub> Buckminsterfullerene", *Journal of the American Chemical Society* **108** (1986) 1301-1302.
9. T. G. Schmalz, W. A. Seitz, D. J. Klein, & G. E. Hite, "Elemental Carbon Cages", *Journal of the American Chemical Society* **110** (1988) 1113-1127.
10. D. J. Klein & N. Trinajstić, "Valence-Bond Theory and Chemical Structure", *Journal of Chemical Education* **67** (1990) 633-637.
11. D. J. Klein & T. G. Schmalz "Buckminsterfullerene, Part A: Introduction" pages 239-246 in *Quasicrystals, Networks, and Molecules of Fivefold Symmetry*, Edited by I. Hargittai (VCH Pub., New York, 1990).
12. D. J. Klein & W. A. Seitz, "Directed Self-Interacting Self-Avoiding Random Walks" pages 403-416 in *Nonlinear Topics in Ocean Physics*, ed. A. R. Osborne (North-Holland, Amsterdam, 1991).
13. D. J. Klein, T. P. Zivkovic, & R. Valenti, "Topological Long-range Order for Resonating Valence-Bond Structures", *Physical Review B* **43** (1991) 723-727.
14. D. J. Klein & X. Liu, "Theorems for Carbon Cages", *Journal of Mathematical Chemistry* **11** (1992) 199-205.
15. D. J. Klein, "Aromaticity *via* Kekulé Structures and Conjugated Circuits", *Journal of Chemical Education* **69** (1992) 691-694.
16. D. J. Klein & M. Randić, "Resistance Distance", *Journal of Mathematical Chemistry* **12** (1993) 81-95.
17. D. J. Klein, T. P. Zivkovic, & A. T. Balaban, "The Fractal Family of Coro<sup>[N]</sup>enes", *Communications in Mathematical Chemistry (MatCh)* **29** (1993) 107-130.
18. H-Y. Zhu, D. J. Klein, W. A. Seitz, & N. H. March, "BN-Alternants: Boron Nitride Cages and Polymers", *Inorganic Chemistry* **34** (1995) 1377-1383.
19. D. J. Klein, "Similarity and Dissimilarity in Posets", *Journal of Mathematical Chemistry* **18** (1995) 321-348.
20. M. A. Garcia-Bach & D. J. Klein, "Cluster-expansion Representation", *Journal of Physics A* **29** (1996) 103-114.
21. L. Bytautas & D. J. Klein, "Alkane Isomer Combinatorics: Stereostructure Enumeration & Graph-Invariant & Molecular-Property Distributions", *Journal of Chemical Information & Computer Sciences* **39** (1999) 803-818.
22. D. J. Klein, "Topo-Graphs, Embeddings, and Molecular Structure" pages 39-83 in *Mathematical Chemistry, vol. 4- Chemical Topology*, ed. D. Bonchev & D.H. Rouvray (Gordon and Breach Pub., NY, 1999).
23. L. Bytautas, D. J. Klein, & T. G. Schmalz, "All acyclic hydrocarbons: formula periodic table and property overlap plots *via* chemical combinatorics", *New Journal of Chemistry* **24** (2000) 329-336.
24. D. J. Klein, "Topo-combinatoric categorization of quasi-local graphitic defects", *Physical Chemistry - Chemical Physics* **4** (2002) 2099-2110.
25. T. Ivanciuc & D. J. Klein, "Parameter-Free Structure-Property Correlation *via* Progressive Reaction Posets for Substituted Benzenes", *Journal of Chemical Information & Computer Sciences* **44** (2004) 610-617.
26. T. Ivanciuc, O. Ivanciuc, & D. J. Klein, "Modeling the bioconcentration factors and bioaccumulation factors of polychlorinated biphenyls with posetic quantitative super-structure/activity relationships (QSSAR)", *Molecular Diversity* **10** (2006) 133-145.
27. A. T. Balaban & D. J. Klein, "Is chemistry 'The Central Science'? How are different sciences related? Co-citations, reductionism, emergence, & posets", *Scientometrics* **69** (2006) 615-637.
28. D. J. Klein, "Defected/decorated benzenoid/graphitic nanostructures", *Pure & Applied Chemistry* **80** (2008) 1399-1414.
29. J. Oliva, D. J. Klein, P. V. R. Schleyer, & L. Serrano-Andres, "Design of Carborane Molecular Architectures with Electronic Structure Computations: From Endohedral and Polyradical Systems to Multidimensional Networks", *Pure & Applied Chemistry* **81** (2009) 719-729.
31. W. Yang, F. Zhang, & D. J. Klein, "Benzenoid Links", *Journal of Mathematical Chemistry* **47** (2010) 457-476.
32. Guillermo Restrepo, Rainer Brüggemann, & Douglas J. Klein, "Partially Ordered Sets: Ranking and Prediction of Substances' Properties", *Current Computer-Aided Drug Design* **7** (2011) 133-145.
33. 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 Journal of Organic Chemistry* **5** (2011) 27-61.
34. D. J. Klein & V. Rosenfeld, "Forcing, Freedom, & Uniqueness in Graph Theory & Chemistry", *Croatica Chemica Acta* **87** (2014) 49-59.