Dr. Detlef W.M. Hofmann

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Education

1987 to 1991 - work on doctoral thesis at the Chair of Theoretical Chemistry under Prof. Dr. Dr. h. c. J. Ladik

1990 - research student at the universities of Rome and Naples (Prof. Dr. Bossa and Prof. Dr. Del Re)

1991 - doctor's degree with the best possible predicate ('mit Auszeichnung')
on the thesis 'Quantum mechanical investigation of conformational solitons in stacked organic systems'

1992 to 1994 - consultant, CRS4, Development and programming of density functional theories in the group of Prof. Clementi, Italy)

1995 to 2002 - research on force fields by data mining, crystal structure prediction and crystal structure determination at the German National Research Center for information technology in the group bioinformatics (Prof T. Lengauer)

2002 to 2004 - teaching, preparation of the habilitation, and scientific work at the University of Frankfurt at the department of inorganic and analytical chemistry in the group of Prof. M.Schmidt.

since 2005 - consultant, CRS4, Italy, investigation in molecular dynamic simulation of hydrogen fuel cells.

Publications by google scholar:

Selected Publications:

1. **L. Pisani, M. Valentini, D.W.M. Hofmann, L.N. Kuleshova, B. D'Aguanno**
   An analytical model for the conductivity of polymeric sulfonated membranes
   Solid State Ionics (2008),179, 465 476

2. **Detlef W.M. Hofmann, Liudmila Kuleshova, Bruno D'Aguanno**
   Molecular dynamics simulation of hydrated Nafion with a reactive force field for water
   J. Mol. Mod. (2008), 14, 225-235

3. **Detlef W.M. Hofmann, Liudmila Kuleshova, Bruno D'Aguanno**
   A new reactive potential for the Molecular Dynamics simulation of liquid water.
   Chem.Phys.Lett. (2007), 448, 138-143

4. **M.U. Schmidt, C. Buchsbaum, J. M. Schnorr, D. W. M. Hofmann, and M. Ermrich**
   Pigment Orange 5: cystal structure determination from a non-indexed X-ray powder diagram
   Z. Krist. (2007), 222, 30-33

5. **M.V. Makarov, L.N.Kuleshova, D.W.M.Hofmann, V.P.Djadchenko,and M.Yu.Antipin**
   Ferrocenylbiphenyl- and Ferrocenylterphenyl- Containing Liquid Crystals: Precursors, Properties and Structures.
   Crystallography Reports. (2006), 51, 792-803

6. **M.U. Schmidt, D.W.M.Hofmann, C. Buchsbaum, and H.J.Metz**
   Crystal Structures of Pigment Red 170 and Derivatives, as Determined by X-ray Powder Diffraction
   Angewandte Chemie Int. Ed. (2006) 45, 1313-1317.

7. **D.W.M.Hofmann and L.N.Kuleshova**
   A Method for Automated Determination of the Crystal Structure from X-ray Powder Diffraction Data
   Crystallography Reports. (2006). 51. 452-460.

8. **D.W.M.Hofmann and L.N.Kuleshova**
A New similarity index for crystal structure determination from X-ray powder diagrams.
Journal of Applied Crystallography (2005) 38, 861-866.

9. **G. M. Day, W. D. S. Motherwell, H. L. Ammon, S. X. M. Boerrigter, R. G. Della Valle, E. Venuti, A. Dzyabchenko, B. P. van Eijck, P. Erk, J. C. Facelli, V. E. Bazterra, M. B. Ferraro, D. W. M. Hofmann, F. J. J. Leusen, C. Liang, C. C. Pantelides, P. G. Karamertzanis, S. L. Price, T. C. Lewis, A. Torrissi, H. Nowell, H. Scheraga, Y. Arnautova, M. U. Schmidt, B. Schweizer, P. Verwer:**
A third blind test of crystal structure prediction,
Acta Cryst B. (2005) 61, 511-527.

10. **D. W. M. Hofmann and L. N. Kuleshova:**
New Force Field for Molecular Simulation and Crystal Design Developed based on the Data Mining Method
Crystallography Reports (2005) 50, 335-337.

11. **C. Schauerte, C. Buchsbaum, L. Fink, D. W. M. Hofmann, M.U. Schmidt, J. Knipping, and R. Boese**
Crystal Structures of trans- and cis-octenes
Acta Cryst (2005). A61, C290-C291

12. **Л.Н. Кулешова, Д.В.М. Хоффманн, М.Ю. Антипин**
Систематические исследования общих закономерностей строения и предсказание кристаллической структуры органических соединений
Журнал Кристаллография (2005) 50, 199-208

13. **D. W. M. Hofmann, L. N. Kuleshova and M.Yu Antipin**
Supramolecular Synthons and Crystal structure prediction of Organic Compounds
Crystal Growth & Design (2004) 4, 1395-1402.

14. **D.W.M. Hofmann**
Crystal Modeling in der organischen und metallorganischen Chemie
Habilitation, Frankfurt a. Main, 2004

15. **L. N. Kuleshova, D. W. M. Hofmann und M. Yu Antipin**
Systematic investigations on general structural features of organic molecular crystals and crystal structure prediction,
Crystallography Reports, 49, 10-19 (2004).

16. **D.W.M. Hofmann and J. Apostolakis**

Crystal structure prediction by data mining
J.Mol.Struc.(Theochem), 647, 17-39 (2003).

17. **D.W.M. Hofmann**
Fast Estimation of Crystal Densities ,
Acta Cryst. B, 58, 489-493 (2002).

18. **W.D.S. Motherwell, H.L. Ammon, A. Dzyabchenko, P. Erk, J.D. Dunitz, A. Gavezzotti, D.W.M. Hofmann, F.J.J. Leusen, J.P.M. Lomerse, W.T.M. Mooij, S.L. Price, H. Scheraga, B. Schweizer, M.U. Schmidt, B.P. van Eijck, P. Verwer, and D.E. Williams:**
Crystal Structure Prediction of Small Organic Molecules: a second blind test,
Acta Cryst, B58, 647-661 (2002).

19. **J. Apostolakis, D.W.M. Hofmann, and T. Lengauer:**
Derivation of a scoring function for crystal structure prediction,
Acta Cryst A, A57, 442-450 (2001).

20. **J. Apostolakis, D.W.M. Hofmann, and T. Lengauer:**
Using sinple learning machines to derive a new potential for molecular modeling
Rational Approaches to drug design, H.-D. Höltje und W.Sippl, Prous Science, Barcelona, 2001, 125-134.

21. **J.P.M. Lommerse, W.D.S. Motherwell, H.L. Ammon, J.D. Dunitz, A. Gavezzotti, D.W.M. Hofmann, F.J.J. Leusen, W.T.M. Mooij, S.L. Price, B. Schweizer, M.U. Schmidt, B.P. van Eijck, P. Verwer, and D.E. Williams:**
A Test of Crystal Structure Prediction of Small Organic Molecules,
Acta Cryst., B56, 697-714 (2000).

22. **D.W.M. Hofmann, and T. Lengauer:**
Prediction of Crystal Structures for Organic Molecules,
J.Mol.Struc.(Theochem) 474, 13-23 (1999).

23. **D.W.M. Hofmann, and T. Lengauer:**
Crystal Structure Prediction based on Statistical Potentials,
J.Mol.Mod. 4, 132-144 (1998).

24. **D.W.M. Hofmann, and T. Lengauer:**
A Discrete Algorithm for Crystal Structure Prediction of Organic Molecules,
Acta Cryst. A53, 225-235 (1997).

25. **Detlef Hofmann, Thomas Lengauer, Christina Oligschleger und Stephan Wefing**
Berechnung von kristallinen und amorphen molekularen Strukturen
Der GMD-Spiegel 2/3, 18-21 (1996).

26. **E. Clementi, and D.W.M Hofmann:**
Coulomb-hole-Hartree-Fock functional for molecular systems.
J. Mol. Struc. (Theochem) 330, 17-31 (1995).

27. **E.Clementi, L. De Windt, and D.W.M Hofmann:**
Extension of the Coulomb-Hole-Hartree-Fock theory to molecules.
Int. J. Quant. Chem. 53, 131 (1995).

28. **E.Clementi, and D.W.M Hofmann:**
Coulomb-Hole-Hartree-Fock Functional,
Int. J. Quant. Chem. 52, 849-865 (1994).

29. **J. Ladik, D.W.M. Hofmann, W. Förner, and P. Otto:**
Investigation of the possibility of solitary waves in the base stacks of DNA.
Physiol. Chem. Phys. & Med. NMR, 24, 227-236 (1992).

30. **D.W.M. Hofmann, J. Ladik, W. Förner, and P. Otto:**
Possibility of solitary waves in the base stacks of DNA.
J. Phys.: Cond. Matter 4, 3883-3903 (1992).

31. **D.W.M. Hofmann, W. Förner, P. Otto, J. Ladik:**
Influence of impurities on soliton dynamics in stacked systems.
J. Phys.: Cond. Matter 2, 4081-4097 (1990).

32. **G. Del Re, W. Förner, D.W.M. Hofmann, and J. Ladik:**
Discrete-state approach to the time evolution of molecular states.
Chem. Phys. 139, 265-281 (1989)

33. **W. Förner, J. Ladik, D.W.M. Hofmann, M. Seel, and A. Godzik, F. Martino:**
Soliton dynamics in alternatingtranspolyacetylene and in stacked systems.
J. Mol. Struct. (Theochem) 188, 231-260 (1989).

34. **D.W.M. Hofmann, W. Förner, and J. Ladik:**
Conformational solitons in stacked systems.

Phys. Rev. A 37, 4429-4438 (1988).

35.

Recent conference contributions

- ***Application of a new similarity index for automatic structure determination and cluster analysis of powder diagrams** (oral contriution).*
  16th Annual Meeting of the German Society for Crystallography, Erlangen, Germany March 3-6, 2008
- ***A New Reactive Force Field, RFF, for the description of the structure and proton transport in water, strong acid solutions and polymeric membranes (poster contribution)***
  Soft, Complex, and Biological Matter Conference, Città del Mare, Terrasini, Sicily, July 15-19, 2007
- ***Theoretical evaluation of structural and dynamical properties of Nafion and composite Nafion membranes (oral contriution)***
  Polymer Batteries-Fuel Cells, PBFC-2007 , Rome, Italy, June 11-14, 2007
- ***New Reactive Force Field for Proton Transport in Water, Acid Solutions and Polymeric Electrolyte Membranes .***
  Conference on "From Physical Understanding to Novel Architectures of Fuel Cells", Trieste, Italy, May 21-25, 2007
- ***Simulation of composite Nafion fuel cell membranes (oral presentation and member of organizing comitee)***
  Proton transport in Polymeric Membranes: Modern Trends in Simulation Methods and Experimental Techniques, Pula, Italy, October 15-18, 2006
- ***A simple analytical model for the conductivity of polymeric sulfonated membranes Molecular Dynamics analysis of hydrated Nafion membranes (poster contribution)*** **Fuel Cells Science & Technology 2006, Sept 13-14, 2006, Turin**
- ***Simulation of composite Nafion fuel cell membranes (oral contriution).***
  6th International Symposium on "New Materials for Electrochemical Systems, July 9-12, 2006, Montreal

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