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Current position:

Senior Scientist, J. Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic, 2004 - present

Previous positions:

- Senior Research Associate, Center for Biological Modeling, Michigan State University, East Lansing, MI, 2002 – 2004
- Postdoctoral Associate with Prof. I.D. Kuntz, Department of Pharmaceutical Chemistry, University of California San Francisco, San Francisco, CA, 2000 – 2002
- Postdoctoral Associate with Prof. K.B. Wiberg, Department of Chemistry, Yale University, New Haven, CT, 1998 – 2000
- Postdoctoral Associate with Prof. Yitzhak Apeloig, Department of Chemistry, Technion - Israel Institute of Technology, Haifa, Israel, 1996 – 1998

Education:

- PhD. in Chemical Physics, Slovak Technical University, Bratislava, Slovak Republic, 1995
- MS with honors in Physical Chemistry, Masaryk University, Brno, Czech Republic, 1990

Research Interests:

We use quantum chemistry as well as DFT methods of solid state physics to model the structure, reactivity, catalytic activity and properties of zeolites.

Prizes, Awards, Honors and Research Fellowships:

- Rector prize for distinction in M.S. Studies, Masaryk University, Brno, Czech Republic 1990
- postdoctoral fellowship, Technion, Haifa, Israel 1996 - 1997
- Purkyne Fellowship, Academy of Sciences of the Czech Republic, Prague, Czech Republic 2004 - 2009

Professional Affiliations:

- American Chemical Society

List of Publications

1. Vladimir Kvasnicka, Stepan Sklenak, Jiri Pospichal: "Neural Network Classification of Inductive and Resonance Effects of Substituents", *J. Am. Chem. Soc.* 1993, 115, 1495.
2. Vladimir Kvasnicka, Stepan Sklenak, Jiri Pospichal: "Application of high-order neural networks in chemistry", *Theor. Chim. Acta* 1993, 86, 257.
3. Vladimir Kvasnicka, Stepan Sklenak, Jiri Pospichal: "Application of Recurrent Neural Networks in Chemistry. Prediction and Classification of ^{13}C NMR Chemical Shifts in a Series of Monosubstituted Benzenes", *J. Chem. Inf. Comput. Sci.* 1992, 32, 742.
4. Vladimir Kvasnicka, Stepan Sklenak, Jiri Pospichal: "Application of neural networks with feedback connections in chemistry: prediction of ^{13}C NMR chemical shifts in a series of monosubstituted benzenes", *Journal of Molecular Structure (THEOCHEM)* 1992, 277, 87.
5. Stepan Sklenak, Vladimir Kvasnicka, Jiri Pospichal: "Prediction of regioselectivity of 1,3-dipolar cycloadditions by neural networks", *Acta Chimica Hungarica - MODELS IN CHEMISTRY* 1993, 130, 103.
6. Vladimir Kvasnicka, Stepan Sklenak, Jiri Pospichal: "Neuronove site pro chemii I. Teorie, software, hardware", *Chemicke Listy* 1993, 87, 79 (Czech).
7. Vladimir Kvasnicka, Stepan Sklenak, Jiri Pospichal: "Neuronove site pro chemii II. Aplikace", *Chemicke Listy* 1993, 87, 157 (Czech).
8. Stepan Sklenak, Vladimir Kvasnicka, Jiri Pospichal: "Prediction of ^{13}C NMR Chemical Shifts by Neural Networks in a Series of Monosubstituted Benzenes", *Chemical Papers*, 1994, 48, 135.
9. Stepan Sklenak, Stanislav Biskupic, Anton Gatial: "Ab initio Study of 4-Azidobutine", *J. Mol. Struct. (THEOCHEM)*, 1995, 336, 75.
10. Anton Gatial, Stepan Sklenak, Peter Klæboe, Claus Jorgen Nielsen, Hanno Priebe, Reiner Salzer and Dana Kurkova: "The infrared and Raman spectra, conformations and ab initio calculations of 4-Azidobut-1-ine", *J. Mol. Struct.*, 1995, 349, 149.
11. Stepan Sklenak, Stanislav Biskupic, Anton Gatial: "Semiempirical study of Methoxy - and (un)Substituted Amino-Methylene-Ethylidene Propandinitriles", *Acta Chimica Hungarica - MODELS IN CHEMISTRY*, 1995, 132, 831.

12. Stepan Sklenak, Stanislav Biskupic, Anton Gatial: "Ab initio study of Methoxy -and (un)Substituted Amino-Methylene-Ethylidene Propandinitriles", *Acta Chimica Hungarica - MODELS IN CHEMISTRY*, 1997, 134, 97.
13. Anton Gatial, Stepan Sklenak, Viktor Milata, Peter Klæboe, Stanislav Biskupic, Dieter Scheller and Jana Juraskova: "The Vibrational Spectra, Conformations and Ab Initio Calculation of Aminomethylene, Propandinitrile and its N-Methyl Derivatives", *Structural Chemistry*, 1996, 7, 17.
14. Stepan Sklenak, Anton Gatial, Stanislav Biskupic: "Ab initio study of Small Organic Azides", *J. Mol. Struct. (THEOCHEM)*, 1997, 397, 249.
15. Anton Gatial, Stepan Sklenak, V. Milata, Stanislav Biskupic, L. Zalibera and Reiner Salzer: "The vibrational and NMR spectra, conformations and ab initio calculations of methoxymethylene- and 1-methoxyethylidene- propanedinitrile", *J. Mol. Struct.*, 1997, 410, 435.
16. Stepan Sklenak, Yitzhak Apeloig, Zvi Rappoport: " Calculated pK(Enol) values for enols of carboxylic acid derivatives $HC=C(OH)X$ ($X = OH, NH_2, NMe_2, OMe, OCHO, F, Cl, Br$)", *J. Am. Chem. Soc.*, 1998, 120, 10359.
17. Uri Zoller, E. Shakkour, Irine Pastersky, Stepan Sklenak, Yitzhak Apeloig: "Polycyclic arene episulfides. Attempted synthesis, molecular orbital calculations and comparison with arene oxides", *TETRAHEDRON*, 1998, 54, 14283.
18. Anton Gatial, Stepan Sklenak, V. Milata, Stanislav Biskupic, Reiner Salzer, Dieter Scheller and G. Woelki: "The vibrational and NMR spectra, conformations and ab initio calculations of 1-aminoethylidene propanedinitrile and its N-methyl derivatives", *J. Mol. Struct.*, 1999, 509, 67.
19. Anton Gatial, Stepan Sklenak, Peter Klæboe, Claus Jorgen Nielsen, Hanno Priebe, Reiner Salzer, Dana Kurkova: "The Vibrational Spectra Including Matrix Isolation, Conformations and ab initio Calculations of 4-Azidobut-1-yne", *J. Mol. Struct.*, 2000, 519, 101.
20. Kenneth B. Wiberg, Stepan Sklenak, William F. Bailey: "Solvation and Structural Effects on the Stability of 10-X-2 Ate Complexes: A Computational Study", *J. Org. Chem.*, 2000, 65, 2014.
21. Jayanta Kumar Mukhopadhyaya, Stepan Sklenak, Zvi Rappoport: "Enols of Carboxylic Acid Amides with β -Electron-Withdrawing Substituents", *J. Am. Chem. Soc.*, 2000, 122, 1325.
22. Yitzhak Apeloig, Stepan Sklenak: "On the Possible Formation of Si=O, Si=S and Si=Se Double Bonds via the Reaction of Silylenes with Oxirane, Thiirane and Selenirane, respectively. An Ab Initio Theoretical Study", *Can. J. Chem.*, 2000, 78, 1496.

23. Stepan Sklenak, Yitzhak Apeloig, Zvi Rappoport: "Calculated equilibria for simple thioenol/thiocarbonyl pairs. Comparison with the oxygen analogs and with the parent Se and Te systems", *J. Chem. Soc. Perk. T. 2*, 2000, 2269.
24. Jayanta Kumar Mukhopadhyaya, Stepan Sklenak and Zvi Rappoport: "Cyano-, Nitro- and Alkoxy-carbonyl-Activated Observable Stable Enols of Carboxylic Acid Amides", *J. Org. Chem.*, 2000, 65, 6856.
25. Kenneth B. Wiberg, Stepan Sklenak, William F. Bailey: "A Computational Study of 10-X-2 Ate Complexes Derived from Vinylolithiums and Vinyl Halides", *Organometallics*, 2001, 20, 771.
26. Henry Castejon, Kenneth B. Wiberg, Stepan Sklenak, Wolfgang Hinz: "Solvent Effects on Methyl Transfer Reactions. 2. The Reaction of Amines with Trimethylsulfonium Salts", *J. Am. Chem. Soc.*, 2001, 123, 6092.
27. Gerhard Maas, Mechthild Alt, Dieter Mayer, Uwe Bergsträßer, Stepan Sklenak, Prince Xavier, Yitzhak Apeloig: "Catalytic and Photochemical Cyclopropanation of Alkenes with Methyl Diazo(trialkylsilyl)acetates: Steric Effects and Thermodynamic Stabilities of Cyclopropanes", *Organometallics*, 2001; 20; 4607.
28. J. Robin Fulton, Stepan Sklenak, Marco W. Bouwkamp, and Robert G. Bergman: "Investigating the Basicity of a Parent Amidoruthenium Complex: Experimental and Computational Results", *J. Am. Chem. Soc.*, 2002, 124, 4722.
29. Stepan Sklenak, Lishan Yao, Robert I. Cukier and Honggao Yan: "Catalytic Mechanism of Yeast Cytosine Deaminase. An ONIOM Computational Study", *J. Am. Chem. Soc.*, 2004, 126, 14879.
30. Lishan Yao, Stepan Sklenak, Honggao Yan and Robert I. Cukier: "A Molecular Dynamics Exploration of the Catalytic Mechanism of Yeast Cytosine Deaminase", *J. Phys. Chem. B*, 2005, 109, 7500.
31. Stepan Sklenak and Jan Hrusak: "CuNO₂ and Cu⁺NO₂ revisited: A comparative ab initio and DFT study", *J. Chem. Theory Comput.*, 2006, 2, 997.
32. Kenneth B. Wiberg, Yi-gui Wang, Stepan Sklenak, Carol Deutsch and Gary Trucks: "Permanganate Oxidation of Alkenes. Substituent and Solvent Effects. Difficulties with MP2 Calculations", *J. Am. Chem. Soc.*, 2006, 128, 11537.
33. Lubomir Benco, Tomas Bucko, Robert Grybos, Juergen Hafner, Zdenek Sobalik, Jiri Dedecek, Stepan Sklenak, and J. Hrusak: "Multiple Adsorption of NO on Fe²⁺ Cations in the

Alpha- and Beta-Positions of Ferrierite: An Experimental and Density Functional Study", *J. Phys. Chem. C.*, 2007, 111, 9393.

34. Stepan Sklenak, Jiri Dedecek, Chengbin Li, Blanka Wichterlova, Vendula Gabova, Marek Sierka and Joachim Sauer: "Aluminum Siting in Silicon-rich Zeolite Frameworks. A Combined High Resolution ^{27}Al NMR and QM/MM Study of ZSM-5", *Angew. Chem., Int. Ed.*, 2007, 46, 7286.

35. Stepan Sklenak, Jiri Dedecek, Chengbin Li, Fei Gao, Bavornpon Jansang, Bundet Boekfa, Blanka Wichterlova, and Joachim Sauer: "Aluminum siting in the ZSM-22 and Theta-1 zeolites revisited: A QM/MM study", *Collect. Czech. Chem. Commun.*, 2008, 73, 909.

36. Stepan Sklenak, Jiri Dedecek, Chengbin Li, Blanka Wichterlova, Vendula Gabova, Marek Sierka, and Joachim Sauer: "Aluminium siting in the ZSM-5 framework by combination of high resolution ^{27}Al NMR and DFT/MM calculations", *Phys. Chem. Chem. Phys.*, 2009, 11, 1237.

37. Jiri Dedecek, Stepan Sklenak, Chengbin Li, Blanka Wichterlova, Vendula Gabova, Jiri Brus, Marek Sierka, and Joachim Sauer: "Effect of Al-Si-Al and Al-Si-Si-Al Pairs in the ZSM-5 Zeolite Framework on the ^{27}Al NMR Spectra. A Combined High-Resolution ^{27}Al NMR and DFT/MM Study", *J. Phys. Chem. C*, 2009, 113, 1447.

38. Kamil Jisa, Jana Novakova, Michal Schwarze, Alena Vondrova, Stepan Sklenak, and Zdenek Sobalik: "Role of the Fe-zeolite structure and iron state in the N_2O decomposition: Comparison of Fe-FER, Fe-BEA, and Fe-MFI catalysts", *J. Catal.*, 2009, 262, 27.

39. Jiri Dedecek, Stepan Sklenak, Chengbin Li, Fei Gao, Jiri Brus, Qingjun Zhu, and Takashi Tatsumi: "Effect of Al/Si Substitutions and Silanol Nests on the Local Geometry of Si and Al Framework Sites in Silicone-Rich Zeolites: A Combined High Resolution ^{27}Al and ^{29}Si NMR and Density Functional Theory/Molecular Mechanics Study", *J. Phys. Chem. C*, 2009, 113, 14454.

40. Stepan Sklenak, Prokopis C. Andrikopoulos, Bundet Boekfa, Bavornpon Jansang, Jana Novakova, Lubomir Benco, Tomas Bucko, Juergen Hafner, Jiri Dedecek, and Zdenek Sobalik: " N_2O decomposition over Fe-zeolites: Structure of the active sites and the origin of the distinct reactivity of Fe-ferrierite, Fe-ZSM-5, and Fe-beta. A combined periodic DFT and multispectral study", *J. Catal.*, 2010, 272, 262.

41. Jiri Dedecek, Melissa J. Lucero, Chengbin Li, Fei Gao, Petr Klein, Martina Urbanova, Zdenka Tvaruzkova, Petr Sazama, and Stepan Sklenak: "Complex Analysis of the Aluminum

Siting in the Framework of Silicon-Rich Zeolites. A Case Study on Ferrierites", J. Phys. Chem. C, 2011, 115, 11056.

42. Petr Sazama, Blanka Wichterlova, Jiri Dedecek, Zdenka Tvaruzkova, Zuzana Musilova, Luisa Palumbo, Stepan Sklenak, Olga Gonsiorova: "FTIR and ^{27}Al MAS NMR analysis of the effect of framework Al- and Si-defects in micro- and micro-mesoporous H-ZSM-5 on conversion of methanol to hydrocarbons", Micropor. Mesopor. Mat., 2011, 143, 87.

43. Jifeng Wang, Stepan Sklenak, Aizhuo Liu, Krzysztof Felczak, Yan Wu, Yue Li, and Honggao Yan: "Role of Glutamate 64 in the Activation of the Prodrug 5-fluorocytosine by Yeast Cytosine Deaminase", Biochemistry, 2012, 51, 475.