

DAFTAR PUSTAKA

- Adams, D.J., Adams, E.M., Hills, G.J., 1979. The Computer Simulation of Polar Liquids. *Mol. Phys.*, 38, 387–400.
- Ahlrichs, R., Bär, M., Häser, M., Horn, H., Kölmel, C., 1989. Electronic Structure Calculations on Workstation Computers: The Program System Turbomole. *Chem. Phys. Lett.*, 162, 165–169.
- Allen, M., Tildesley, D., 1987. *Computer Simulation of Liquids*. Oxford University Press, New York.
- Appl, M., 2000. Ammonia, 1. Introduction. In: Ullmann's Encyclopedia of Industrial Chemistry. Wiley-VCH Verlag GmbH & Co. KGaA.
- Armunanto, R., Schwenk, C.F., Randolph, B.R., Rode, B.M., 2004a, Ag(I) Ion in Liquid Ammonia. *Chem. Phys. Lett.*, 388, 395–399.
- Armunanto, R., Schwenk, C.F., Rode, B.M., 2003, Structure and Dynamics of Hydrated Ag(I): Ab Initio Quantum Mechanical-Molecular Mechanical Molecular Dynamics Simulation, *J. Phys. Chem. A*, 107, 3132–3138.
- Armunanto, R., Schwenk, C.F., Tran, H.T., Rode, B.M., 2004b, Structure and Dynamics of Au⁺ Ion in Aqueous Solution: Ab Initio QM/MM MD Simulations, *J. Am. Chem. Soc.*, 126, 2582–2587.
- Azam, S.S., Hofer, T.S., Randolph, B.R., Rode, B.M., 2009. Hydration of Sodium(I) and Potassium(I) Revisited: A Comparative QM/MM and QMCF MD Simulation Study of Weakly Hydrated Ions, *J. Phys. Chem. A*, 113, 1827–34.
- Bakowies, D., Thiel, W., 1996, Hybrid Models for Combined Quantum Mechanical and Molecular Mechanical Approaches, *J. Phys. Chem.*, 3654, 10580–10594.
- Bene, G.E., Hofer, T.S., Randolph, B.R., Rode, B.M., 2012, Simulation of Electronic Excitation in the Liquid State by Quantum Mechanical Charge Field Molecular Dynamics, *Chem. Phys. Lett.*, 521, 74–77.
- Berendsen, H.J.C., Postma, J.P.M., van Gunsteren, W.F., DiNola, A., Haak, J.R., 1984, Molecular Dynamics with Coupling to an External Bath, *J. Chem. Phys.*, 81, 3684–3690.
- Bopp, P., 1986, A Study of the Vibrational Motions of Water in an Aqueous CaCl₂ Solution, *Chem. Phys.*, 106, 205–212.

- Boys, S.F., Bernardi, F., 1970, The Calculation of Small Molecular Interactions by the Differences of Separate Total Energies. Some Procedures with Reduced Errors, *Mol. Phys.*, 19, 553–566.
- Brode, S., Horn, H., Ehrig, M., Moldrup, D., Rice, J.E., Ahlrichs, R., 1993, Parallel Direct SCF and Gradient Program for Workstation Clusters, *J. Comput. Chem.*, 14, 1142–1148.
- Canaval, L.R., Weiss, A.K.H., Rode, B.M., 2013, Structure and Dynamics of the Th⁴⁺-Ion in Aqueous Solution – An Ab Initio QMCF-MD Study, *Comput. Theor. Chem.*, 1022, 94–102.
- Dunning, T.H., 1970, Gaussian Basis Functions for Use in Molecular Calculations. I. Contraction of (9s5p) Atomic Basis Sets for the First-Row Atoms, *J. Chem. Phys.*, 53, 2823–2833.
- Famulari, A., Moroni, F., Raimondi, M., Thorsteinsson, T., 2001, The Structure of Lithium and Potassium Cations Coordinated by Ammonia Molecules in the Gas Phase as Revealed by Ab Initio SCF-MI Calculations, *J. Mol. Struct. THEOCHEM*, 549, 85–93.
- Field, M.J., Bash, P.A., Karplus, M., 1990, A Combined Quantum Mechanical and Molecular Mechanical Potential for Molecular Dynamics Simulations, *J. Comput. Chem.*, 11, 700–733.
- Frisch, M.J., Trucks, G.W., Schlegel, H.B., Scuseria, G.E., Robb, M.A., Cheeseman, J.R., Scalmani, G., Barone, V., Mennucci, B., Petersson, G.A., Nakatsuji, H., Caricato, M., Li, X., Hratchian, H.P., Izmaylov, A.F., Bloino, J., Zheng, G., Sonnenberg, J.L., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Montgomery Jr., J.A., Peralta, J.E., Ogliaro, F., Bearpark, M., Heyd, J.J., Brothers, E., Kudin, K.N., Staroverov, V.N., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A., Burant, J.C., Iyengar, S.S., Tomasi, J., Cossi, M., Rega, N., Millam, J.M., Klene, M., Knox, J.E., Cross, J.B., Bakken, V., Adamo, C., Jaramillo, J., Gomperts, R., Stratmann, R.E., Yazyev, O., Austin, A.J., Cammi, R., Pomelli, C., Ochterski, J.W., Martin, R.L., Morokuma, K., Zakrzewski, V.G., Voth, G.A., Salvador, P., Dannenberg, J.J., Dapprich, S., Daniels, A.D., Farkas, Ö., Foresman, J.B., Ortiz, J. V, Cioslowski, J., Fox, D.J., 2009. Gaussian 09 Revision D.01.
- Gardiner, D.J., 1973, Infrared and Raman Spectra of Lithium and Ammonium Nitrate Solutions in Liquid Ammonia, *J. Chem. Phys.*, 59, 175.
- Hannongbua, S., 1998, On the Solvation of Lithium Ions in Liquid Ammonia: Monte Carlo Simulations with a Three-Body Potential, *Chem. Phys. Lett.*, 288, 663–668.

- Hannongbua, S., Kokpol, S., Gurskii, Z., Heinzinger, K., 1997, Cluster Formation in a Concentrated Lithium-Liquid Ammonia Solution. A Monte Carlo Study. *Z. Naturforsch.*, 52a, 828–834.
- Hannongbua, S., Remsungnen, T., Kiselev, M., Heinzinger, K., 2003, The Structure of Concentrated Li-Ammonia Solutions as Derived from MD Simulations., *Condens. Matter Phys.*, 6, 459–470.
- Hannongbua, S.V., Ishida, T., Spohr, E., Heinzinger, K., 1988, Molecular Dynamics Study of a Lithium Ion in Ammonia, *Z. Naturforsch.*, 582, 572–582.
- Hayama, S., Skipper, N.T.N., Wasse, J.C., Thompson, H., 2002, X-Ray Diffraction Studies of Solutions of Lithium in Ammonia: The Structure of the Metal–nonmetal Transition, *J. Chem. Phys.*, 116, 2991–2996.
- Hofer, T.S., 2014, Perspectives for Hybrid Ab Initio/molecular Mechanical Simulations of Solutions: From Complex Chemistry to Proton-Transfer Reactions and Interfaces, *Pure Appl. Chem.*, 86, 105.
- Hofer, T.S., Pribil, A.B., Randolph, B.R., Rode, B.M., 2005, Structure and Dynamics of Solvated Sn(II) in Aqueous Solution: An Ab Initio QM/MM MD Approach, *J. Am. Chem. Soc.*, 127, 14231–14238.
- Hofer, T.S., Randolph, B.R., Rode, B.M., 2008, The Hydration of the Mercury(I)-Dimer – A Quantum Mechanical Charge Field Molecular Dynamics Study, *Chem. Phys.*, 349, 210–218.
- Hofer, T.S., Randolph, B.R., Rode, B.M., 2008a, Al(III) Hydration Revisited. An Ab Initio Quantum Mechanical Charge Field Molecular Dynamics Study, *J. Phys. Chem. B*, 112, 11726–33.
- Hofer, T.S., Randolph, B.R., Rode, B.M., 2008b, *Solvation Effects on Molecules and Biomolecules*, Springer Netherlands, Dordrecht.
- Hofer, T.S., Tran, H.T., Schwenk, C.F., Rode, B.M., 2004, Characterization of Dynamics and Reactivities of Solvated Ions by Ab Initio Simulations, *J. Comput. Chem.*, 25, 211–217.
- Hofer, T.S., Weiss, A.K.H., Randolph, B.R., Rode, B.M., 2011, Hydration of Highly Charged Ions, *Chem. Phys. Lett.*, 512, 139–145.
- Humphrey, W., Dalke, A., Schulten, K., 1996, VMD Visual Molecular Dynamics, *J. Mol. Graph.*, 14, 33–38.
- Kaye, G.W.C., Laby, T.H., 1995, *Tables of Physical and Chemical Constants*, 16th ed. Longmann, London.

- Kerdcharoen, T., Liedl, K., Rode, B., 1996, A QM/MM Simulation Method Applied to the Solution of Li^+ in Liquid Ammonia, *Chem. Phys.*, 211, 313–323.
- Kritayakornpong, C., 2008, The Jahn-Teller Effect of the Ag^{2+} Ion in Aqueous Solution : A Hybrid Ab Initio Quantum Mechanical / Molecular Mechanical Molecular Dynamics Simulation, *Chem. Phys. Lett.*, 455, 207–212.
- Leach, A.R., 2001, *Molecular Modelling PRINCIPLES AND APPLICATIONS Second Edition*, Second. ed. Pearson Education, Great Britain.
- Loeffler, H.H., Mohammed, A.M., Inada, Y., Funahashi, S., 2003, Lithium(I) Ion Hydration: A QM/MM-MD Study., *Chem. Phys. Lett.*, 379, 452–457.
- Loeffler, H.H., Rode, B.M., 2002, The Hydration Structure of the Lithium Ion, *J. Chem. Phys.*, 117, 110–117.
- Loutellier, a., Manceron, L., Perchard, J.P., 1990, An Infrared Study of Lithium-Ammonia and Potassium-Ammonia Complexes Trapped in Solid Argon, *Chem. Phys.*, 146, 179–193.
- Lutz, O.M.D., Hofer, T.S., Randolf, B.R., Weiss, A.K.H., Rode, B.M., 2012, A QMCF-MD Investigation of the Structure and Dynamics of Ce^{4+} in Aqueous Solution, *Inorg. Chem.*, 51, 6746–52.
- Maeda, K., Lodge, M.T.J., Harmer, J., Freed, J.H., Edwards, P.P., 2012, Electron Tunneling in Lithium-Ammonia Solutions Probed by Frequency-Dependent Electron Spin Relaxation Studies, *J. Am. Chem. Soc.*, 134, 9209–18.
- Mierzwicki, K., Latajka, Z., 2001. Nonadditivity of Interaction in $\text{Li}(\text{NH}_3)_n$ and $\text{Li}(\text{NH}_3)_n^+$ ($n=1-4$) Clusters. *Chem. Phys.*, 265, 301–311.
- Motherwell, W., Zuberi, S., 2006, Observations on the Reductive Ring Opening Reactions of Alkylidenecyclopropyl Ketones Promoted by Lithium in Liquid Ammonia, *Tetrahedron Lett.*, 47, 8789–8791.
- Mulliken, R.S., 1955, Electronic Population Analysis on LCAO–MO Molecular Wave Functions, I. *J. Chem. Phys.*, 23, 1833.
- Orabi, E., Lamoureux, G., 2013, Molecular Dynamics Investigation of Alkali Metal Ions in Liquid and Aqueous Ammonia, *J. Chem. Theory Comput.*, 9, 2324–2338.
- Pranowo, H.D., Rode, B.M., 1999, Solvation of Cu^{2+} in Liquid Ammonia: Monte Carlo Simulation Including Three-Body Corrections, *J. Phys. Chem. A*, 103, 4298–4302.

- Ramachandran, K.I., Deepa, G., Namboori, K., 2008, *Computational Chemistry and Molecular Modelling: Principles and Application*, Springer-Verlag, Berlin.
- Randolf, B.R., 2010, *Simulations of Liquids and Solutions Based on Quantum Mechanical Forces*, Advances In Inorganic Chemistry - Volume 62, Elsevier Inc.
- Rode, B.M., Hofer, T.S., Randolf, B.R., Schwenk, C.F., Xenides, D., Vchirawongkwin, V., 2005, Ab Initio Quantum Mechanical Charge Field (QMCF) Molecular Dynamics: A QM/MM – MD Procedure for Accurate Simulations of Ions and Complexes, *Theor. Chem. Acc.*, 115, 77–85.
- Rode, B.M., Schwenk, C.F., Hofer, T.S., Randolf, B.R., 2005, Coordination and Ligand Exchange Dynamics of Solvated Metal Ions, *Coord. Chem. Rev.*, 249, 2993–3006.
- Sripa, P., Tongraar, A., Kerdcharoen, T., 2013, “Structure-Making” Ability of Na⁺ in Dilute Aqueous Solution : An ONIOM-XS MD Simulation Study, *J. Phys. Chem. A*, 117, 1826–1833.
- Stephenson, J., 2006, Highly Functionalized and Soluble Multiwalled Carbon Nanotubes by Reductive Alkylation and Arylation: The Billups Reaction, *Chem. Mater.*, 4658–4661.
- Thompson, H., Wasse, J.C., Skipper, N.T., Hayama, S., Bowron, D.T., Soper, A.K., 2003, Structural Studies of Ammonia and Metallic Lithium-Ammonia Solutions, *J. Am. Chem. Soc.*, 125, 2572–81.
- Tirler, A.O., Weiss, A.K.H., Hofer, T.S., 2013, A Comparative Quantum Mechanical Charge Field Study of Uranyl Mono- and Dicarboxylate Species in Aqueous Solution, *J. Phys. Chem. B*, 117, 16174–87.
- Tongraar, A., Hannongbua, S., 2008, Solvation Structure and Dynamics of Ammonium NH₄⁺ in Liquid Ammonia Studied by HF/MM and B3LYP/MM Molecular Dynamics Simulations, *J. Phys. Chem. B*, 112, 885–891.
- Tongraar, A., Kerdcharoen, T., Hannongbua, S., 2006, Simulations of Liquid Ammonia Based on the Combined Quantum Mechanical/molecular Mechanical (QM/MM) Approach, *J. Phys. Chem. A*, 110, 4924–4929.
- Tongraar, A., Liedl, K.R., Rode, B.M., 1998, The Hydration Shell Structure of Li⁺ Investigated by Born-Oppenheimer Ab Initio QM/MM Dynamics, *Chem. Phys. Lett.*, 286, 56–64.
- Tongraar, A., Rode, B.M., 1999, Preferential Solvation of Li⁺ in 18.45 % Aqueous Ammonia : A Born-Oppenheimer Ab Initio Quantum Mechanics/Molecular

Mechanics MD Simulation, *J. Phys. Chem. A*, 103, 8524–8527.

Tongraar, A., Rode, B.M., 2008, The Role of Second Shell Quantum Effects on the Preferential Solvation of Li^+ in Aqueous Ammonia: An Extended Ab Initio QM/MM MD Simulation with Enlarged QM Region, *Chem. Phys. Lett.*, 466, 61–64.

Wasse, J., Hayama, S., Skipper, N., Fischer, H., 2000, Structure of a Metallic Solution of Lithium in Ammonia, *Phys. Rev. B*, 61, 11993-11997.

Wasse, J.C., Hayama, S., Masmanidis, S., Stebbings, S.L., Skipper, N.T., 2003, The Structure of Lithium–ammonia and Sodium–ammonia Solutions by Neutron Diffraction, *J. Chem. Phys.*, 118, 7486–7494.

Weiss, A.K.H., Hofer, T.S., 2013, Exploiting the Capabilities of Quantum Chemical Simulations to Characterise the Hydration of Molecular Compounds, *RSC Adv.*, 3, 1606.

Zurek, E., Edwards, P.P., Hoffmann, R., 2009, A Molecular Perspective on Lithium-Ammonia Solutions, *Angew. Chem. Int. Ed. Engl.*, 48, 8198–232.

Zvilichovsky, G., Gbara-Haj-Yahia, I., 2004, Birch Reduction of (-)-Ephedrine. Formation of a New, Versatile Intermediate for Organic Synthesis, *J. Org. Chem. Note*, 5490–5493.