

**2019**

151. E.E. Bruce, N.F.A. van der Vegt

**Molecular scale solvation in complex solutions**

J. Am. Chem. Soc. 141, 12948-12956 (2019) JACS Perspective

150. D. Rosenberger, N.F.A. van der Vegt

**Relative entropy indicates an ideal concentration for structure-based coarse graining of binary mixtures**

Phys. Rev. E 99, 053308 (2019)

149. S. Bharadwaj, N.F.A. van der Vegt

**Does preferential adsorption drive cononsolvency?**

Macromolecules 52, 4131-4138 (2019)

148. D. Rosenberger, T. Sanyal, M.S. Shell, N.F.A. van der Vegt

**Transferability of local density-assisted implicit solvation models for homogeneous fluid mixtures**

J. Chem. Theory Comput. 15, 2881-2895 (2019)

147. C. Dalgicdir, N.F.A. van der Vegt

**Improved temperature behavior of PNIPAM in water with a modified OPLS model**

J. Phys. Chem. B 123, 3875-3883 (2019)

146. E.E. Bruce, P.T. Bui, B.A. Rogers, P.S. Cremer, N.F.A. van der Vegt

**Nonadditive ion effects drive both collapse and swelling of thermoresponsive polymers in water**

J. Am. Chem. Soc. 141, 6609-6616 (2019)

145. G. Deichmann, N.F.A. van der Vegt

**Conditional reversible work coarse-grained models with explicit electrostatics – An application to butylmethylimidazolium ionic liquids**

J. Chem. Theory Comput. 15, 1187-1198

144. G. Deichmann, M. Dallavalle, D. Rosenberger, N.F.A. van der Vegt

**Phase equilibria modeling with systematically coarse-grained models – A comparative study on state point transferability**

J. Phys. Chem. B 123, 504-515 (2019)

143. T. Pfeiffer, A. De Nicola, C. Montis, F. Carla, N.F.A. van der Vegt, D. Berti, G. Milano

**Nanoparticles at biomimetic interfaces: Combined experimental and simulation study on charged gold nanoparticles/lipid bilayer interfaces**

J. Phys. Chem. Lett. 10, 129-137 (2019)

**2018**

142. G. Deichmann, N.F.A. van der Vegt

**Bottom-up approach to represent dynamic properties in coarse-grained molecular simulations**

J. Chem. Phys. 149, 244114 (2018)

141. E.E. Bruce, N.F.A. van der Vegt

**Does an electronic continuum correction improve effective short-range ion-ion interactions in aqueous solution?**

J. Chem. Phys. 148, 222816 (2018)

140. I.M. Ilie, D. Nayar, W.K. den Otter, N.F.A. van der Vegt, W.J. Briels

**Intrinsic conformational preferences and interactions in  $\alpha$ -synuclein fibrils: Insights from molecular dynamics simulations**

J. Chem. Theory Comp. 14, 3298-3310 (2018)

139. D. Nayar, N.F.A. van der Vegt

**Cosolvent effects on polymer hydration drive polymer collapse**

J. Phys. Chem. B 122, 3587-3596 (2018)

138. J. Milzetti, D. Nayar, N.F.A. van der Vegt

**Convergence of Kirkwood-Buff integrals of ideal and nonideal aqueous solutions using molecular dynamics simulations**

J. Phys. Chem. B 122, 5515-5526 (2018)

137. D. Rosenberger, N.F.A. van der Vegt

**Addressing the temperature transferability of structure based coarse graining models**

Phys. Chem. Chem. Phys. 20, 6617-6628 (2018)

136. P. Ganguly, P. Boserman, N.F.A. van der Vegt, J.-E. Shea

**TMAO counteracts urea denaturation by inhibiting protein-urea preferential interaction**

J. Am. Chem. Soc. 140, 483-492 (2018)

## 2017

135. G. Deichmann, N.F.A. van der Vegt

**Conditional reversible work coarse-grained models of molecular liquids with Coulomb electrostatics – A proof of concept study on weakly polar organic molecules**

J. Chem. Theory Comp. 13, 6158-6166 (2017)

134. N.F.A. van der Vegt, D. Nayar

**The hydrophobic effect and the role of cosolvents**

J. Phys. Chem. B 121, 9986-9998 (2017) Feature Article (ACS editor's choice)

133. M. Dallavalle, N.F.A. van der Vegt

**Evaluation of mapping schemes for systematic coarse graining of higher alkanes**

Phys. Chem. Chem. Phys. 19, 23034-23042 (2017)

132. C. Dalgicdir, F. Rodríguez-Ropero, N.F.A. van der Vegt

**Computational calorimetry of PNIPAM cononsolvency in water/methanol mixtures**

J. Phys. Chem. B 121, 7741-7748 (2017)

131. D. Nayar, A. Folberth, N.F.A. van der Vegt

**Molecular origin of urea driven hydrophobic polymer collapse and unfolding depending on side chain chemistry**

Phys. Chem. Chem. Phys. 19, 18156-18161 (2017)

130. N.F.A. van der Vegt, F. Rodríguez-Ropero

**Comment on “Relating side chain organization of PNIPAm with its conformation in aqueous methanol” by D. Mukherji et al., Soft Matter, 2016, 12, 7995**

Soft Matter 13, 2289-2291 (2017)

## 2016

129. D. Rosenberger, M. Hanke, N.F.A. van der Vegt

**Comparison of iterative inverse coarse-graining methods**

Eur. Phys. J. Spec. Top. 225, 1323-1345 (2016)

128. R. Zhang, N.F.A. van der Vegt

**Study of hydrophobic clustering in partially sulfonated polystyrene solutions with a systematic coarse-grained model**

Macromolecules 49, 7571-7580 (2016)

127. K. Rane, N.F.A. van der Vegt

**Using grand canonical Monte Carlo simulations to understand the role of interfacial fluctuations on solvation at the water–vapor Interface**

J. Phys. Chem. B 120, 9697-9707 (2016)

126. F. Rodríguez-Ropero, P. Rötzscher, N.F.A. van der Vegt

**Comparison of different TMAO force fields and their impact on the folding equilibrium of a hydrophobic polymer**

J. Phys. Chem. B 120, 8757-8767 (2016) Correction: J. Phys. Chem. B 121, 1455-1455 (2017)

125. P. Ganguly, N.F.A. van der Vegt, J.-E. Shea

**Hydrophobic association in mixed urea-TMAO solutions**

J. Phys. Chem. Lett. 7, 3052-3059 (2016)

124. F. Taherian, V. Marcon, E. Bonaccorso, N.F.A. van der Vegt

**Vortex formation in coalescence of droplets with a reservoir using molecular dynamics simulations**

J. Colloid Interf. Sci. 479, 189-198 (2016)

123. N.F.A. van der Vegt, K. Haldrup, S. Roke, J. Zheng, M. Lund, H. J. Bakker

**Water-mediated ion pairing: Occurrence and relevance**

Chem. Rev. 116, 7626-7641 (2016)

122. K. Rane, N.F.A. van der Vegt

**Understanding the influence of capillary waves on solvation at the liquid-vapor interface**  
J. Chem. Phys. 144, 114111 (2016)

121. F. Taherian, F. Leroy, L.-O. Heim, E. Bonaccorso, N.F.A. van der Vegt

**Mechanism for asymmetric nanoscale electrowetting of an ionic liquid on graphene**  
Langmuir 32, 140-150 (2016)

## 2015

120. F. Rodríguez-Ropero, T. Hajari, N.F.A. van der Vegt

**Mechanism of polymer collapse in miscible good solvents**

J. Phys. Chem. B 119, 15780-25788 (2015)

119. V. R. Ardham, G. Deichmann, N.F.A. van der Vegt, F. Leroy

**Solid-liquid work of adhesion of coarse-grained models of n-hexane on graphene layers derived from the conditional reversible work method**

J. Chem. Phys. 143, 243135 (2015)

118. M. A. Pérez-Maciá, D. Curcó, R. Bringué, M. Iborra, F. Rodríguez-Ropero, N.F.A. van der Vegt, C. Alemán

**1-Butanol absorption in poly(styrene-divinylbenzene) ion exchange resins for catalysis**

Soft Matter 11, 9144-9149 (2015)

117. F. Taherian, F. Leroy, N.F.A. van der Vegt

**Interfacial tension does not drive asymmetric electrowetting on graphene**

Langmuir 31, 4686-4695 (2015)

116. T. Hajari, N.F.A. van der Vegt

**Solvation thermodynamics of amino acid side chains on a short peptide backbone**

J. Chem. Phys. 142, 144502 (2015)

115. F. Rodríguez-Ropero, N.F.A. van der Vegt

**On the urea induced hydrophobic collapse of a water soluble polymer**

Phys. Chem. Chem. Phys. 17, 8491-8498 (2015)

114. P. Ganguly, T. Hajari, J.-E. Shea, N.F.A. van der Vegt

**Mutual exclusion of urea and trimethylamine N-oxide from amino acids in mixed solvent environment**

J. Phys. Chem. Lett. 6, 581-585 (2015) Correction: J. Phys. Chem. Lett. 6, 4728-4729 (2015)

## 2014

113. G. Deichmann, V. Marcon, N.F.A. van der Vegt

**Bottom-up derivation of conservative and dissipative interactions for coarse-grained molecular liquids with the conditional reversible work method**

J. Chem. Phys. 141, 224109 (2014)

112. V. Marcon, N.F.A. van der Vegt

**How does low-molecular-weight polystyrene dissolve: Osmotic swelling vs. surface dissolution**

Soft Matter 10, 9059-9064 (2014)

111. T. Hajari, N.F.A. van der Vegt

**Peptide backbone effect on hydration free energies of amino acid side chains**

J. Phys. Chem. B 118, 13162-13168 (2014)

110. F. Rodríguez-Ropero, N.F.A. van der Vegt

**Direct osmolyte-macromolecule interactions confer entropic stability to folded states**

J. Phys. Chem. B 118, 7327-7334 (2014)

109. P. Ganguly, T. Hajari, N.F.A. van der Vegt

**Molecular simulation study of Hofmeister cations and the aqueous solubility of benzene**

J. Phys. Chem. B 118, 5331-5339 (2014)

## 2013

108. P. Ganguly, N.F.A. van der Vegt

**Representability and transferability of Kirkwood-Buff iterative Boltzmann inversion models for multicomponent aqueous systems**

J. Chem. Theory Comput. 9, 5247-5256 (2013)

107. F. Taherian, F. Leroy, N.F.A. van der Vegt

**Interfacial entropy of water at rigid hydrophobic surfaces**

Langmuir 29, 9807-9813 (2013)

106. C.R. Herbers, C. Li, N.F.A. van der Vegt

**Grand challenges in quantum-classical modeling of molecule-surface interactions**

J. Comput. Chem. 34, 1177-1188 (2013)

105. J.-W. Shen, C. Li, N.F.A. van der Vegt, C. Peter

**Understanding the control of mineralization by polyelectrolyte additives: Simulation of preferential binding to calcite surfaces**

J. Phys. Chem. C 117, 6904-6913 (2013)

104. F. Taherian, V. Marcon, N.F.A. van der Vegt, F. Leroy

**What is the contact angle of water on graphene?**

Langmuir 29, 1457-1465 (2013)

103. P. Ganguly, N.F.A. van der Vegt

**Convergence of sampling Kirkwood-Buff integrals of aqueous solutions with molecular dynamics simulations**

J. Chem. Theory Comput. 9, 1347-1355 (2013)

102. E. Brini, E.A. Algaer, P. Ganguly, C. Li, F. Rodríguez-Ropero, N.F.A. van der Vegt

**Systematic coarse-graining methods for soft matter simulations – a review**

Soft Matter 9, 2108-2119 (2013)

101. F. Rodríguez-Ropero, N.F.A. van der Vegt

**Ionic specific effects on the structure, mechanics and interfacial softness of a polyelectrolyte brush**

Faraday Discuss. 160, 297-309 (2013)

100. L. Chen, C. Li, N.F.A. van der Vegt, G.K. Auernhammer, E. Bonaccorso

**Initial electrospraying of aqueous electrolyte drops**

Phys. Rev. Lett. 110, 026103 (2013)

## 2012

99. E. Brini, N.F.A. van der Vegt

**Chemically transferable coarse-grained potentials from conditional reversible work calculations**

J. Chem. Phys. 137, 154113 (2012)

98. H. A. Karimi-Varzaneh, N.F.A. van der Vegt, F. Müller-Plathe, P. Carbone

**How good are coarse-grained polymer models? A comparison for atactic polystyrene**

ChemPhysChem 13, 3428-3439 (2012)

97. T. Hajari, P. Ganguly, N.F.A. van der Vegt

**Enthalpy–entropy of cation association with the acetate anion in water**

J. Chem. Theory Comput. 8, 3804-3809 (2012)

96. D. Mukherji, N.F.A. van der Vegt, K. Kremer

**Preferential solvation of triglycine in aqueous urea: An open boundary simulation approach**

J. Chem. Theory Comput. 8, 3536-3541 (2012)

95. K. Johnston, C. R. Herbers, N.F.A. van der Vegt

**Development of classical molecule–surface interaction potentials based on density functional theory calculations: Investigation of force field representability**

J. Phys. Chem. C 116, 19781-19788 (2012)

94. E. Brini, C. R. Herbers, G. Deichmann, N.F.A. van der Vegt

**Thermodynamic transferability of coarse-grained potentials for polymer–additive systems**

Phys. Chem. Chem. Phys. 14, 11896-11903 (2012)

93. P. Ganguly, D. Mukherji, C. Junghans, N.F.A. van der Vegt

**Kirkwood–Buff coarse-grained force fields for aqueous solutions**

J. Chem. Theory Comput. 8, 1802-1807 (2012)

92. C. Li, J. Shen, C. Peter, N.F.A. van der Vegt

**A chemically accurate implicit-solvent coarse-grained model for polystyrenesulfonate solutions**

Macromolecules 45, 2551-2561 (2012)

91. V. Marcon, D. Fritz, N.F.A. van der Vegt  
**Hierarchical modelling of polystyrene surfaces**  
Soft Matter 8, 5585-5594 (2012)

90. D. Mukherji, N.F.A. van der Vegt, K. Kremer, L. Delle Site  
**Kirkwood–Buff analysis of liquid mixtures in an open boundary simulation**  
J. Chem. Theory Comput. 8, 375-379 (2012)

89. L. Delle Site, C. Holm, N.F.A. van der Vegt  
**Multiscale approaches and perspectives to modeling aqueous electrolytes and polyelectrolytes**  
Top. Curr. Chem. 307, 251-294 (2012)

## 2011

88. E. Algaer, N.F.A. van der Vegt  
**Hofmeister ion interactions with model amide compounds**  
J. Phys. Chem. B 115, 13781-13787 (2011)

87. D. Fritz, K. Koschke, V. A. Harmandaris, N.F.A. van der Vegt, K. Kremer  
**Multiscale modeling of soft matter: scaling of dynamics**  
Phys. Chem. Chem. Phys. 13, 10412-10420 (2011)

86. E. Brini, V. Marcon, N.F.A. van der Vegt  
**Conditional reversible work method for molecular coarse graining applications**  
Phys. Chem. Chem. Phys. 13, 10468-10474 (2011)

85. S. Chen, X. Huang, W. Wen, P. Sheng, N.F.A. van der Vegt  
**Microscopic mechanism of the giant electrorheological effect**  
Int. J. Mod. Phys. B 25, 7 897-903 (2011)

84. P. Ganguly, P. Schravendijk, B. Hess, N.F.A. van der Vegt  
**Ion pairing in aqueous electrolyte solutions with biologically relevant anions**  
J. Phys. Chem. B 115, 3734-3739 (2011)

83. C.R. Herbers, K. Johnston, N.F.A. van der Vegt  
**Modelling molecule–surface interactions—an automated quantum-classical approach using a genetic algorithm**  
Phys. Chem. Chem. Phys. 13, 10577-10583 (2011)

82. J.-W. Shen, C. Li, N.F.A. van der Vegt, C. Peter  
**Transferability of coarse grained potentials: Implicit solvent models for hydrated ions**  
J. Chem. Theory Comput. 7, 1916-1927 (2011)

## 2010

81. S. Chen, X. Huang, N.F.A. van der Vegt, W. Wen, P. Sheng

**Giant electrorheological effect: A microscopic mechanism**

Phys. Rev. Lett. 105, 046001 (2010)

80. S. Neyertz, D. Brown, S. Pandiyan, N.F.A. van der Vegt

**Carbon dioxide diffusion and plasticization in fluorinated polyimides**

Macromolecules 43, 7813-7827 (2010)

79. S. Pandiyan, D. Brown, S. Neyertz, N.F.A. van der Vegt

**Carbon dioxide solubility in three fluorinated polyimides studied by molecular dynamics simulations**

Macromolecules 43, 2605-2621 (2010)

78. A. Villa, C. Peter, N.F.A. van der Vegt

**Transferability of nonbonded interaction potentials for coarse-grained simulations: Benzene in water**

J. Chem. Theory Comput. 6, 2434-2444 (2010)

77. N.F.A. van der Vegt, V. A. Kusuma, B.D. Freeman

**Basis of solubility versus Tc correlations in polymeric gas separation membranes**

Macromolecules 43, 1473-1479 (2010)

## 2009

76. D. Fritz, C. R. Herbers, K. Kremer, N.F.A. van der Vegt

**Hierarchical modeling of polymer permeation**

Soft Matter 5, 4556 (2009)

75. D. Fritz, V. A. Harmandaris, K. Kremer, N.F.A. van der Vegt

**Coarse-grained polymer melts based on isolated atomistic chains: Simulation of polystyrene of different tacticities**

Macromolecules 42, 7579 (2009)

74. B. Hess, N.F.A. van der Vegt

**Cation specific binding with protein surface charges**

Proc. Natl. Acad. Sci. USA 106, 13296 (2009)

73. S. Pandiyan, D. Brown, N.F.A. van der Vegt, S. Neyertz

**Atomistic models of three fluorinated polyimides in the amorphous state**

J. Polym. Sci. Part B: Polym. Phys. 47, 1166 (2009)

72. A. Villa, N.F.A. van der Vegt, C. Peter

**Self-assembling dipeptide: Including solvent degrees of freedom in a coarse-grained model**

Phys. Chem. Chem. Phys. 11, 2068 (2009)

71. A. Villa, C. Peter, N.F.A. van der Vegt

**Self-assembling dipeptides: Conformational sampling in solvent-free coarse-grained simulation**  
Phys. Chem. Chem. Phys. 11, 2077 (2009)

70. B. Hess, J. A. W. Harings, S. Rastogi, N.F.A. van der Vegt

**Interaction of water with N, N'-1,2-ethanediyl-bis(6-hydroxy-hexanamide) crystals: A simulation study**

J. Phys. Chem. B 113, 627 (2009)

69. T. Mulder, V. A. Harmandaris, A. V. Lyulin, N.F.A. van der Vegt, K. Kremer, M.A.J. Michels  
**Structural properties of atactic polystyrene of different thermal history obtained from a multi-scale simulation**

Macromolecules 42, 384 (2009)

## 2008

68. T. Mulder, V.A. Harmandaris, A.V. Lyulin, N.F.A. van der Vegt, M.A.J. Michels  
**Molecular simulation via connectivity-altering Monte Carlo and scale-jumping methods: Application to amorphous polystyrene**  
Macromol. Theory Sim. 17, 393 (2008)

67. B. Hess, N.F.A. van der Vegt  
**Predictive modeling of phenol chemical potentials in molten bisphenol-A-polycarbonate over a broad temperature range**  
Macromolecules 41, 7281 (2008)

66. L.M. Ghiringhelli, B. Hess, N.F.A. van der Vegt, L. Delle Site  
**Competing adsorption between hydrated peptides and water onto metal surfaces: from electronic to conformational properties**  
J. Am. Chem. Soc. 130, 13460 (2008)

65. N.F.A. van der Vegt, C. Peter, K. Kremer  
**Structure-based coarse- and fine-graining in soft matter simulations**  
In Gregory A. Voth, editor, Coarse Graining of Condensed Phase and Biomolecular Systems , chapter 25, p.379-397, Chapman and Hall/CRC Press, Taylor and Francis Group, 2008

64. T. Mulder, V.A. Harmandaris, A.V. Lyulin, N.F.A. van der Vegt, B. Vorselaars, M.A.J. Michels  
**Equilibration and deformation of amorphous polystyrene: Scale-jumping simulation approach**  
Macromol. Theory Sim. 17, 290 (2008)

63. T.A. Ozal, C. Peter, B. Hess, N.F.A. van der Vegt  
**Modeling solubilities of additives in polymer microstructures: Single-step perturbation method based on a soft-cavity reference state**  
Macromolecules 41, 5055 (2008)

62. B. Hess, C. Peter, T. Ozal, N.F.A. van der Vegt

**Fast growth thermodynamic integration: Calculating excess chemical potentials of additive molecules in polymer microstructures**

Macromolecules 41, 2283 (2008)

**2007**

61. B. Hess, N.F.A. van der Vegt

**Solvent-averaged potentials for alkali-, earth alkali- and alkylammonium halide aqueous solutions**

J. Chem. Phys. 127, 234508 (2007)

60. V.A. Harmandaris, N.P. Adhikari, N.F.A. van der Vegt, K. Kremer, B.A. Mann, R. Voelkel, H. Weiss,

C. Liew

**Ethylbenzene diffusion in polystyrene: United atom atomistic/coarse grained simulations and experiments**

Macromolecules 40, 7026 (2007)

59. V.A. Harmandaris, D. Reith, N.F.A. van der Vegt, K. Kremer

**Comparison between coarse-graining models for polymer systems: Two mapping schemes for polystyrene**

Macromol. Chem. Phys. 208, 2109 (2007)

58. C. Peter, N.F.A. van der Vegt

**Solvent reorganization contributions in solute transfer thermodynamics: Inferences from the solvent equation of state**

J. Phys. Chem. B 111, 7836 (2007)

57. D. Trzesniak, N.F.A. van der Vegt, W.F. van Gunsteren

**Analysis of neo-pentane-urea potentials of mean force in aqueous urea**

Mol. Phys. 105, 33 (2007)

56. P. Schravendijk, L.M. Ghiringhelli, L. Delle Site, N.F.A. van der Vegt

**Interaction of hydrated amino acids with metal surfaces: A multiscale modeling description**

J. Phys. Chem. C 111, 2631 (2007)

55. M.-E. Lee, N.F.A. van der Vegt

**Molecular thermodynamics of methane solvation in tert-butanol-water mixtures**

J. Chem. Theory Comput. 3, 194 (2007)

54. W.F. van Gunsteren, D.P. Geerke, C. Oostenbrink, D. Trzesniak, N.F.A. van der Vegt

**Analysis of driving forces for biomolecular solvation and association.** In: „Protein Folding and Drug Design“

Proceedings of the International School of Physics „Enrico Fermi“ (R.A. Broglia and G. Tiana, eds.)  
165, pp. 177-191 (2007), IOS Press, Amsterdam, and SIF, Bologna

**2006**

53. V.A. Harmandaris, N.P. Adhikari, N.F.A. van der Vegt, K. Kremer

**Hierarchical modeling of polystyrene: From atomistic to coarse grained simulations**

Macromolecules 39, 6708 (2006)

52. B. Hess, N.F.A. van der Vegt

**Hydration thermodynamic properties of amino acid analogs: A systematic comparison of biomolecular force fields and water models**

J. Phys. Chem. B 110, 17616 (2006)

51. N.F.A. van der Vegt, M.-E. Lee, D. Trzesniak, W.F. van Gunsteren

**Enthalpy-entropy compensation in the effects of urea on hydrophobic interactions**

J. Phys. Chem. B 110, 12852 (2006)

50. T.A. Ozal, N.F.A. van der Vegt

**Confusing cause and effect: Energy-entropy compensation in the preferential solvation of a nonpolar solute in dimethyl sulfoxide/water mixtures**

J. Phys. Chem. B 110, 12104 (2006)

49. W.F. van Gunsteren, D. Bakowies, R. Baron, I. Chandrasekhar, M. Christen, X. Daura, P. Gee, D.P. Geerke, A. Glättli, P.H. Hünenberger, M.A. Kastenholz, C. Oostenbrink, M. Schenk, D. Trzesniak, N.F.A. van der Vegt, H.B. Yu

**Biomolecular modelling: Goals, problems, perspectives**

Angewandte Chemie Int. Ed. 45, 4064 (2006)

48. B. Hess, C. Holm, N.F.A. van der Vegt

**Osmotic coefficients of atomistic NaCl (aq) force fields**

J. Chem. Phys. 124, 164509 (2006)

47. B. Hess, S. Leon, N.F.A. van der Vegt, K. Kremer

**Long time atomistic trajectories from coarse grained simulations: Bisphenol-A polycarbonate**

Soft Matter 2, 409 (2006)

46. B. Hess, C. Holm, N.F.A. van der Vegt

**Modeling multibody effects in ionic solutions with a concentration dependent dielectric permittivity**

Phys. Rev. Lett. 96, 147801 (2006)

45. M.-E. Lee, N.F.A. van der Vegt

**Does urea denature hydrophobic interactions?**

J. Am. Chem. Soc. 128, 4948 (2006)

44. V. Marcon, N.F.A. van der Vegt, G. Wegner, G. Raos

**Modeling of molecular packing and conformation in oligofluorenes**

J. Phys. Chem. B 110, 5253 (2006)

2005

43. S. Leon, N.F.A. van der Vegt, L. Delle Site, K. Kremer

**Bisphenol-A polycarbonate: Entanglement analysis from coarse-grained MD simulations**

Macromolecules 38, 8078 (2005)

42. P. Schravendijk, N.F.A. van der Vegt, L. Delle Site, K. Kremer

**Dual-scale modeling of benzene adsorption onto Ni(111) and Au(111) surfaces in explicit water**

ChemPhysChem 6, 1866 (2005)

41. P. Schravendijk, N.F.A. van der Vegt

**From hydrophobic to hydrophilic solvation: An application to hydration of benzene**

J. Chem. Theory Comput. 1, 643 (2005)

40. C. Oostenbrink, T.A. Soares, N.F.A. van der Vegt, W.F. van Gunsteren

**Validation of the 53A6 GROMOS force field**

Eur. Biophys. J. 34, 273 (2005)

39. M.-E. Lee, N.F.A. van der Vegt

**A new force field for atomistic simulations of aqueous tertiary butanol solutions**

J. Chem. Phys. 122, 114509 (2005)

38. J.N. Barsema, N.F.A. van der Vegt, G.H. Koops, M. Wessling

**Ag-functionalized carbon molecular-sieve membranes based on polyelectrolyte/polyimide blend precursors**

Adv. Func. Mater. 15, 69 (2005)

**2004**

37. D.M. Sterescu, L. Bolhuis-Versteeg, N.F.A. van der Vegt, D.F. Stamatialis, M. Wessling

**Novel gas separation membranes containing covalently bonded fullerenes**

Macromol. Rapid Commun. 25, 1674 (2004)

36. J.N. Barsema, S.D. Klijnstra, J. H. Balster, N.F.A. van der Vegt, G.H. Koops, M. Wessling

**Intermediate polymer to carbon gas separation membranes based on Matrimid PI**

J. Membrane Sci. 238, 93 (2004)

35. G.F. Hermans , M. Wessling, N.F.A. van der Vegt

**Polymer intrusion into narrow pores at the interface between a poor solvent and adsorbing and non-adsorbing surfaces**

Polymer 45, 3027 (2004)

34. D. Trzesniak, N.F.A. van der Vegt, W.F. van Gunsteren

**Computer simulation studies on the solvation of aliphatic hydrocarbons in 6.9 M aqueous urea solution**

Phys. Chem. Chem. Phys. 6, 697 (2004) Correction: Phys. Chem. Chem. Phys. 6, 4375 (2004)

33. D.P. Geerke, C. Oostenbrink, N.F.A. van der Vegt, W.F. van Gunsteren  
**An effective force field for molecular dynamics simulations of dimethyl sulfoxide and dimethyl sulfoxide-water mixtures**  
J. Phys. Chem. B 108, 1436 (2004)
32. N.F.A. van der Vegt, D. Trzesniak, B. Kasumaj, W.F. van Gunsteren  
**Energy-entropy compensation in the transfer of nonpolar solutes from water to cosolvent/water mixtures**  
ChemPhysChem 5, 144 (2004) Correction: ChemPhysChem 6, 1010 (2005)

31. N.F.A. van der Vegt, W.F. van Gunsteren  
**Entropic contributions in cosolvent binding to hydrophobic solutes in water**  
J. Phys. Chem. B 108, 1056 (2004)

30. N.F.A. van der Vegt  
**New perspectives on gas sorption in solution-diffusion membranes**  
in Advanced Materials for Membrane Separations Chapter 3, p. 39-54; ACS Symposium Series 876, Eds. I. Pinna, B.D. Freeman, Oxford University Press (2004).

## 2003

29. S.J. Metz, N.F.A. van der Vegt, M.H.V. Mulder, M. Wessling  
**Thermodynamics of water sorption in poly(ethylene oxide) poly(butylene terephthalate) block copolymers**  
J. Phys. Chem. B 107, 13629 (2003)

28. G.F. HermSEN, N.F.A. van der Vegt, M. Wessling  
**Monte Carlo calculations of polymer adsorption at the entrance of cylindrical pores in flat adsorbing surfaces**  
Soft Materials 1, 295 (2003)

27. J.N. Barsema, J. Balster, V. Jordan, N.F.A. van der Vegt, M. Wessling  
**Functionalized Carbon Molecular Sieve membranes containing Ag-nanoclusters**  
J. Membrane Sci. 219, 47 (2003)

26. J.N. Barsema, G.C. Kaptaidakis, N.F.A. van der Vegt, G.H. Koops, M. Wessling  
**Preparation and characterization of highly selective dense and hollow fiber asymmetric membranes based on BTDA-TDI/MDI co-polyimide**  
J. Membrane Sci. 216, 195 (2003)

## 2002

25. B. Krause, G.H. Koops, N.F.A. van der Vegt, M. Wessling, M. Wübbenhorst, J. van Turnhout  
**Ultralow-k dielectrics made by supercritical foaming of thin polymer films**  
Adv. Mater. 14, 1041 (2002)

24. F.G. Wilhelm, N.F.A. van der Vegt, H. Strathmann, M. Wessling  
**Current-voltage behavior of bipolar membranes in concentrated salt solutions investigated with chronopotentiometry**  
J. Appl. Electrochem. 32, 455 (2002)

23. G.F. Hermsen, B.A. de Geeter, N.F.A. van der Vegt, M. Wessling  
**Monte Carlo simulation of partially confined flexible polymers**  
Macromolecules 35, 5267 (2002)

22. J.N. Barsema, N.F.A. van der Vegt, G.H. Koops, M. Wessling  
**Carbon molecular sieve membranes prepared from porous fiber precursor**  
J. Membrane Sci. 205, 239 (2002)

21. N.F.A. van der Vegt  
**A molecular dynamics simulation study of solvation thermodynamical quantities of gases in polymeric solvents**  
J. Membrane Sci. 205, 125 (2002)

20. B. Krause, N.F.A. van der Vegt, M. Wessling  
**New ways to produce porous polymeric membranes by carbon dioxide foaming**  
Desalination 144, 5 (2002)

19. B. Krause, M. Kloth, N.F.A. van der Vegt, M. Wessling  
**Porous monofilaments by continuous solid state foaming**  
Ind. Eng. Chem. Res. 41, 1195 (2002)

18. F.G. Wilhelm, I.G.M. Pünt, N.F.A. van der Vegt, H. Strathmann, M. Wessling  
**Cation permeable membranes from blends of sulfonated poly (ether ether ketone) and poly (ether sulfone)**  
J. Membrane Sci. 199, 167 (2002)

17. F.G. Wilhelm, N.F.A. van der Vegt, H. Strathmann, M. Wessling  
**Comparison of bipolar membranes by means of chronopotentiometry**  
J. Membrane Sci. 199, 177 (2002)

16. B. Krause, K. Diekmann, N.F.A. van der Vegt, M. Wessling  
**Open nanoporous morphologies from polymeric blends by carbon dioxide foaming**  
Macromolecules 35, 1738 (2002)

15. F.G. Wilhelm, I. Pünt, N.F.A. van der Vegt, H. Strathmann, M. Wessling  
**Asymmetric bipolar membranes in acid-base electrodialysis**  
Ind. Eng. Chem. Res. 41, 579 (2002)

## 2001

14. N.F.A. van der Vegt, F. Müller-Plathe, A. Geleßus, D. Johannsmann

**Orientation of liquid crystal monolayers on polyimide alignment layers: a molecular dynamics simulation study**

J. Chem. Phys. 115, 9935 (2001)

13. B. Krause, H.J.P. Sijbesma, P. Münüklü, N.F.A. van der Vegt, M. Wessling

**Bicontinuous nanoporous polymers by carbon dioxide foaming**

Macromolecules 34, 8792 (2001)

12. B. Krause, M.E. Boerrigter, N.F.A. van der Vegt, H. Strathmann, M. Wessling

**Novel open-cellular polysulfone morphologies produced with trace concentrations of solvent as pore opener**

J. Membrane Sci. 187, 181 (2001)

11. B. Krause, R. Mettinkhof, N.F.A. van der Vegt, M. Wessling

**Microcellular foaming of amorphous high-T-g polymers using carbon dioxide**

Macromolecules 34, 874 (2001)

10. F.G. Wilhelm, N.F.A. van der Vegt, M. Wessling, H. Strathmann

**Chronopotentiometry for advanced current-voltage characterization of bipolar membranes**

J. Electroanal. Chem. 502, 152 (2001)

9. F.G. Wilhelm, I. Pünt, N.F.A. van der Vegt, M. Wessling, H. Strathmann

**Optimization strategies for the preparation of bipolar membranes with reduced salt ion leakage in acid-base electrodialysis**

J. Membrane Sci. 182, 13 (2001)

**2000**

8. F.G. Wilhelm, N.F.A. van der Vegt, M. Wessling, H. Strathmann

**Bipolar membrane preparation**

Chapter 4 in Handbook on Bipolar Membrane Technology, Ed. A.J.B. Kemperman, Twente University Press, 2000, pp. 79-108.

7. J.P. Hoogenboom, H.L. Tepper, N.F.A. van der Vegt, W.J. Briels

**Transport diffusion of argon in AlPO<sub>4</sub>-5 from equilibrium molecular dynamics simulations**

J. Chem. Phys. 113, 6875 (2000)

6. N.F.A. van der Vegt

**Temperature dependence of gas transport in polymer melts: Molecular dynamics simulations of CO<sub>2</sub> in polyethylene**

Macromolecules 33, 3153 (2000)

**1999**

5. H.L. Tepper, J.P. Hoogenboom, N.F.A. van der Vegt, W.J. Briels

**Unidirectional diffusion of methane in AlPO<sub>4</sub>-5**

J. Chem. Phys. 110, 11511 (1999)

4. N.F.A. van der Vegt, W.J. Briels, M. Wessling, H. Strathmann

**The sorption induced glass transition in amorphous glassy polymers**

J. Chem. Phys. 110, 11061 (1999)

**1998**

3. N.F.A. van der Vegt, W.J. Briels

**Efficient sampling of solvent free energies in polymers**

J. Chem. Phys. 109, 7578 (1998)

2. N.F.A. van der Vegt, W.J. Briels, M. Wessling, H. Strathmann

**A nonequilibrium simulation method for calculating tracer diffusion coefficients of small solutes in n-alkane liquids and polymers**

J. Chem. Phys. 108, 9558 (1998)

**1996**

1. N.F.A. van der Vegt, W.J. Briels, M. Wessling, H. Strathmann

**Free energy calculations of small molecules in dense amorphous polymers. Effect of initial guess configuration in molecular dynamics studies**

J. Chem. Phys. 105, 8849 (1996)