

List of publications of Dezső Boda

- [1] D. Boda. *Complexity in Nature and Society. From Dancing Molecules to Collapsing Societies*. iASK Monographs. iASK, 2020.
- [2] D. Boda, M. Valiskó, and D. Gillespie. Modeling the Device Behavior of Biological and Synthetic Nanopores with Reduced Models. *Entropy*, 22(11):1259, 2020. IF: 2.494.
- [3] D. Fertig, M. Valiskó, and D. Boda. Rectification of bipolar nanopores in multivalent electrolytes: effect of charge inversion and strong ionic correlations. *Phys. Chem. Chem. Phys.*, 22(34):19033–19045, 2020. IF: 3.567.
- [4] D. Fertig, D. Boda, and I. Szalai. Brownian dynamics simulation of chain formation in electrorheological fluids. *Hung. J. Ind. Chem.*, 48(1):95–107, 2020.
- [5] B. Hohl, E. Má dai, D. Boda, and M. Valiskó. Modeling of a pH-tunable dual-response nanopore sensor. *J. Mol. Liq.*, 310:112946, 2020. IF: 4.513.
- [6] D. Fertig, B. Matejczyk, M. Valiskó, D. Gillespie, and D. Boda. Scaling Behavior of Bipolar Nanopore Rectification with Multivalent Ions. *J. Phys. Chem. C*, 123(47):28985–28996, 2019. IF:4.484. #Refs = 1.
- [7] E. Má dai, M. Valiskó, and D. Boda. Application of a bipolar nanopore as a sensor: rectification as an additional device function. *Phys. Chem. Chem. Phys.*, 21:19772–19784, 2019. IF: 3.567.
- [8] D. Fertig, M. Valiskó, and D. Boda. Controlling ionic current through a nanopore by tuning pH: a Local Equilibrium Monte Carlo study. *Mol. Phys.*, 117(20):2793–2801, 2019. IF: 1.704.
- [9] M. Valiskó, B. Matejczyk, Z. Ható, T. Kristóf, E. Má dai, D. Fertig, , D. Gillespie, and D. Boda. Multiscale analysis of the effect of surface charge pattern on a nanopore’s rectification and selectivity properties: from all-atom model to Poisson-Nernst-Planck. *J. Chem. Phys.*, 150(14):144703, 2019. IF: 2.843. #Refs = 4.
- [10] E. Má dai, M. Valiskó, and D. Boda. The effect of the charge pattern on the applicability of a nanopore as a sensor. *J. Mol. Liq.*, 283:391–398, 2019. IF: 4.513. #Refs = 1.
- [11] E. Má dai, B. Matejczyk, A. Dallos, M. Valiskó, and D. Boda. Controlling ion transport through nanopores: modeling transistor behavior. *Phys. Chem. Chem. Phys.*, 20(37):24156–24167, 2018. IF: 3.906. #Refs = 1.
- [12] M. Valiskó, T. Kristóf, D. Gillespie, and D. Boda. A systematic Monte Carlo simulation study of the primitive model planar electrical double layer over an extended range of concentrations, electrode charges, cation diameters and valences. *AIP Advances*, 8(2):025320, 2018. IF: 1.568. #Refs = 9.
- [13] D. Fertig, E. Má dai, M. Valiskó, and D. Boda. Simulating ion transport with the NP+LEMC method. Applications to ion channels and nanopores. *Hung. J. Ind. Chem.*, 45(1):73–84, 2017. IF: –.
- [14] E. Má dai, M. Valiskó, A. Dallos, and D. Boda. Simulation of a model nanopore sensor: Ion competition underlines device behavior. *J. Chem. Phys.*, 147(24):244702, 2017. IF: 2.965. #Refs = 1.
- [15] Z. Ható, M. Valiskó, T. Kristóf, D. Gillespie, and D. Boda. Multiscale modeling of a rectifying bipolar nanopore: explicit-water versus implicit-water simulations. *Phys. Chem. Chem. Phys.*, 17(27):17816–17826, 2017. IF: 4.123. #Refs = 2.

- [16] B. Matejczyk, M. Valiskó, M.-T. Wolfram, J.-F. Pietschmann, and D. Boda. Multiscale modeling of a rectifying bipolar nanopore: Comparing Poisson-Nernst-Planck to Monte Carlo. *J. Chem. Phys.*, 146(12):124125, 2017. IF: 2.965. #Refs = 4.
- [17] M. Valiskó and D. Boda. Activity coefficients of individual ions in LaCl_3 from the II+IW theory. *Mol. Phys.*, 115(9–12):1245–1252, 2017. IF: 1.837. #Refs = 7.
- [18] Z. Ható, D. Boda, D. Gillespie, J. Vrabec, G. Rutkai, and T. Kristóf. Simulation study of a rectifying bipolar ion channel: detailed model versus reduced model. *Cond. Matt. Phys.*, 19(1):13802, 2016. IF: 0.748.
- [19] M. Valiskó and D. Boda. Comment on “The Role of Concentration Dependent Static Permittivity of Electrolyte Solutions in the Debye–Hückel Theory”. *J. Phys. Chem. B*, 119(44):14332–14336, 2015. IF: 3.377. #Refs = 7.
- [20] T. Nagy, D. Henderson, and D. Boda. Correction to “Simulation of an electrical double layer model with a low dielectric layer between the electrode and the electrolyte”. *J. Phys. Chem. B*, 119(35):11967–11968, 2015. IF: 3.377.
- [21] M. Valiskó and D. Boda. Unraveling the behavior of the individual ionic activity coefficients on the basis of the balance of ion-ion and ion-water interactions. *J. Phys. Chem. B*, 119(4):1546–1557, 2015. IF: 3.377. #Refs = 15.
- [22] D. Boda, G. Leaf, J. Fonseca, and B. Eisenberg. Energetics of ion competition in the DEKA selectivity filter of neuronal sodium channels. *Cond. Matt. Phys.*, 18(1):13601, 2015. IF: 0.771.
- [23] C. Berti, S. Furini, D. Gillespie, D. Boda, R. S. Eisenberg, E. Sangiorgi, and C. Fiegna. A 3-D Brownian Dynamics simulator for the study of ion permeation through membrane pores. *J. Chem. Theor. Comput.*, 10(8):2911–2926, 2014. IF: 5.215. #Refs = 9.
- [24] M. Valiskó and D. Boda. The effect of concentration- and temperature-dependent dielectric constant on the activity coefficient of NaCl electrolyte solutions. *J. Chem. Phys.*, 140(23):234508, 2014. IF: 3.333. #Refs = 22.
- [25] D. Boda. Monte Carlo Simulation of Electrolyte Solutions in Biology: In and Out of Equilibrium. volume 10 of *Ann. Rep. Comp. Chem.*, chapter 5, pages 127–163. Elsevier, 2014. #Refs = 6.
- [26] D. Boda, É. Csányi, D. Gillespie, and T. Kristóf. Dynamic Monte Carlo simulation of coupled transport through a narrow multiply-occupied pore. *J. Phys. Chem. C*, 118(1):700–707, 2014. IF: 4.805. #Refs = 4.
- [27] D. Boda, R. Kovács, D. Gillespie, and T. Kristóf. Selective transport through a model calcium channel studied by Local Equilibrium Monte Carlo simulations coupled to the Nernst-Planck equation. *J. Mol. Liq.*, 189:100, 2014. IF: 1.580. #Refs = 2.
- [28] D. Boda and D. Gillespie. Calculating the electrostatic potential profiles of double layers from simulation ion density profiles. *Hung. J. Ind. Chem.*, 41(2):125–132, 2013. IF: -. #Refs = 2.
- [29] D. Boda, M. Valiskó, and I. Szalai. The origin of the interparticle potential of electrorheological fluids. *Cond. Matt. Phys.*, 16(4):43002, 2013. IF: 0.811.
- [30] M. Valiskó, D. Henderson, and D. Boda. Selective adsorption of ions in charged slit-systems. *Cond. Matt. Phys.*, 16(4):43601, 2013. IF: 0.811. #Refs = 2.
- [31] D. Boda, D. Henderson, and D. Gillespie. The role of solvation in the binding selectivity of the L-type calcium channel. *J. Chem. Phys.*, 139(5):055103, 2013. IF: 3.333. #Refs = 7.

- [32] Z. Ható, D. Boda, and T. Kristóf. Simulation of steady-state diffusion: Driving force ensured by Dual Control Volumes or Local Equilibrium Monte Carlo. *J. Chem. Phys.*, 137(5):054109, 2012. IF: 3.164. #Refs = 4.
- [33] T. Kristóf, D. Boda, and I. Szalai. An analytic solution for the magnetization of two-dimensional ferrofluids based on the mean spherical approximation. *J. Phys.-condens. Matt.*, 24(33):336002, 2012. IF: 2.355. #Refs = 1.
- [34] R. Kovács, M. Valiskó, and D. Boda. Monte Carlo simulation of the electrical properties of electrolytes adsorbed in charged slit-systems. *Cond. Matt. Phys.*, 15(2):23803, 2012. IF: 0.800. #Refs = 6.
- [35] D. Boda and D. Gillespie. Steady state electrodiffusion from the Nernst-Planck equation coupled to Local Equilibrium Monte Carlo simulations. *J. Chem. Theor. Comput.*, 8(3):824–829, 2012. IF: 5.389. #Refs = 14.
- [36] É. Csányi, D. Boda, D. Gillespie, and T. Kristóf. Current and selectivity in a model sodium channel under physiological conditions: Dynamic Monte Carlo simulations. *Biochim. et Biophys. Acta - Biomembranes*, 1818(3):592–600, 2012. IF: 3.389. #Refs = 20.
- [37] T. Nagy, D. Henderson, and D. Boda. Simulation of an electrical double layer model with a low dielectric layer between the electrode and the electrolyte. *J. Phys. Chem. B*, 115(39):11409–11419, 2011. IF: 3.696. #Refs = 29.
- [38] D. Boda, D. Henderson, B. Eisenberg, and D. Gillespie. A method for treating the passage of a charged hard sphere ion as it passes through a sharp dielectric boundary. *J. Chem. Phys.*, 135(6):064105, 2011. IF: 3.333. #Refs = 6.
- [39] T. Nagy, M. Valiskó, D. Henderson, and D. Boda. The Behavior of 2:1 and 3:1 Electrolytes at Polarizable Interfaces. *J. Chem. Eng. Data*, 56(4):1316–1322, 2011. IF: 1.693. #Refs = 3.
- [40] D. Henderson and D. Boda. Mean spherical approximation for the Yukawa fluid radial distribution function. *Mol. Phys.*, 109(7–10):1009–1013, 2011. IF: 1.819. #Refs = 6.
- [41] J. Vincze, M. Valiskó, and D. Boda. Response to “Comment on ‘The nonmonotonic concentration dependence of the mean activity coefficient of electrolytes is a result of a balance between solvation and ion-ion correlations’ [J. Chem. Phys. 134, 157101 (2011)]”. *J. Chem. Phys.*, 134(15):157102, 2011. IF: 3.333. #Refs = 2.
- [42] Z. Máté, I. Szalai, D. Boda, and D. Henderson. Heat capacities of the dipolar Yukawa model polar fluid. *Mol. Phys.*, 109(2):203–208, 2011. IF: 1.819. #Refs = 7.
- [43] D. Boda, J. Giri, D. Henderson, B. Eisenberg, and D. Gillespie. Analyzing the components of the free energy landscape in a calcium selective ion channel by Widom’s particle insertion method. *J. Chem. Phys.*, 134(5):055102, 2011. IF: 3.333. #Refs = 7.
- [44] J. Giri, J. Fonseca, D. Boda, D. Henderson, and B. Eisenberg. Self-organized models of selectivity in calcium channels. *Phys. Biol.*, 8(2):026004, 2011. IF: 2.595. #Refs = 4.
- [45] J. Vincze, M. Valiskó, and D. Boda. The nonmonotonic concentration dependence of the mean activity coefficient of electrolytes is a result of a balance between solvation and ion-ion correlations. *J. Chem. Phys.*, 133(15):154507, 2010. IF: 2.920. #Refs = 42.
- [46] M. Malasics, D. Boda, M. Valiskó, D. Henderson, and D. Gillespie. Simulations of calcium channel block by trivalent ions: Gd^{3+} competes with permeant ions for the selectivity filter. *Biochim. et Biophys. Acta - Biomembranes*, 1798(11):2013–2021, 2010. IF: 4.647. #Refs = 18.

- [47] G. Rutkai, D. Boda, and T. Kristóf. Relating binding affinity to dynamical selectivity from dynamic Monte Carlo simulations of a model calcium channel. *J. Phys. Chem. Lett.*, 1(14):2179–2184, 2010. IF: 1.592. #Refs = 7.
- [48] A. Malasics and D. Boda. An efficient iterative grand canonical Monte Carlo algorithm to determine individual ionic chemical potentials in electrolytes. *J. Chem. Phys.*, 132(24):244103, 2010. IF: 2.920. #Refs = 11.
- [49] M. Valiskó, T. Varga, A. Baczoni, and D. Boda. The structure of strongly dipolar hard sphere fluids with extended dipoles by Monte Carlo simulations. *Mol. Phys.*, 108(1):87–96, 2010. IF: 1.743. #Refs = 7.
- [50] A. Malasics, D. Gillespie, W. Nonner, D. Henderson, B. Eisenberg, and D. Boda. Protein structure and ionic selectivity in calcium channels: Selectivity filter size, not shape, matters. *Biochim. et Biophys. Acta - Biomembranes*, 1788(12):2471–2480, 2009. IF: 3.998. #Refs = 14.
- [51] M. Valiskó and D. Boda. Correction to the Clausius-Mosotti equation: the dielectric constant of non-polar fluids from Monte Carlo simulations. *J. Chem. Phys.*, 131(16):064120, 2009. IF: 3.093. #Refs = 5.
- [52] D. Boda, M. Valiskó, D. Henderson, B. Eisenberg, D. Gillespie, and W. Nonner. Ion selectivity in L-type calcium channels by electrostatics and hard-core repulsion. *J. Gen. Physiol.*, 133(5):497–509, 2009. IF: 4.260. #Refs = 23.
- [53] Y. He, D. Gillespie, D. Boda, I. Vlasiouk, R. S. Eisenberg, and Z. S. Siwy. Tuning transport properties of nanofluidic devices with local charge inversion. *JACS*, 131(14):5194–5202, 2009. IF: 8.580. #Refs = 154.
- [54] D. Henderson and D. Boda. Insights from theory and simulation on the electrical double layer. *Phys. Chem. Chem. Phys.*, 11(20):3822–3830, 2009. IF: 4.116. #Refs = 67.
- [55] D. Boda, M. Valiskó, D. Henderson, D. Gillespie, B. Eisenberg, and M. K. Gilson. Ions and inhibitors in the binding site of HIV Protease: Comparison of Monte Carlo simulations and the linearized Poisson-Boltzmann theory. *Biophys. J.*, 96(4):1293–1306, 2009. IF: 4.390. #Refs = 6.
- [56] D. Boda and D. Henderson. The effects of deviations from Lorentz-Berthelot rules on the properties of a simple mixture. *Mol. Phys.*, 106(20):2367–2370, 2008. IF: 1.478. #Refs = 65.
- [57] D. Gillespie and D. Boda. The anomalous mole fraction effect in calcium channels: A measure of preferential selectivity. *Biophys. J.*, 95(6):2658–2672, 2008. IF: 4.683. #Refs = 29.
- [58] D. Gillespie, D. Boda, Y. He, P. Apel, and Z.S. Siwy. Synthetic nanopores as a test case for ion channel theories: The anomalous mole fraction effect without single filing. *Biophys. J.*, 95(2):609–619, 2008. IF: 4.683. #Refs = 33.
- [59] A. Malasics, D. Gillespie, and D. Boda. Simulating prescribed particle densities in the grand canonical ensemble using iterative algorithms. *J. Chem. Phys.*, 128(12):124102, 2008. IF: 3.149. #Refs = 20.
- [60] D. Boda, W. Nonner, D. Henderson, B. Eisenberg, and D. D. Gillespie. Volume exclusion in calcium selective channels. *Biophys. J.*, 94(9):3486–3496, 2008. IF: 4.683. #Refs = 13.
- [61] D. Di Caprio, M. Valiskó, M. Holovko, and D. Boda. Simple extension of a field theory approach for the description of the double layer accounting for excluded volume effects. *J. Phys. Chem. C*, 111(43):15700–15705, 2007. IF: -. #Refs = 3.
- [62] M. Valiskó, D. Boda, and D. Gillespie. Selective adsorption of ions with different diameter and valence at highly-charged interfaces. *J. Phys. Chem. C*, 111(43):15575–15585, 2007. IF: -. #Refs = 51.

- [63] D. Boda, M. Valiskó, B. Eisenberg, W. Nonner, D. Henderson, and D. Gillespie. The effect of the protein dielectric coefficient and pore radius on the Na^+ affinity of a model sodium channel. *Biophys. J.*, pages 609A–609A, January 2007. #Refs = 1.
- [64] D. Boda, W. Nonner, M. Valiskó, D. Henderson, B. Eisenberg, and D. Gillespie. Steric selectivity in Na channels arising from protein polarization and mobile side chains. *Biophys. J.*, 93(6):1960–1980, 2007. IF: 4.627. #Refs = 51.
- [65] D. Boda, M. Valiskó, B. Eisenberg, W. Nonner, D. Henderson, and D. Gillespie. Combined effect of pore radius and protein dielectric coefficient on the selectivity of a calcium channel. *Phys. Rev. Lett.*, 98(16):168102, 2007. IF: 6.944. #Refs = 33.
- [66] M. Valiskó, D. Henderson, and D. Boda. The capacitance of the electrical double layer of valence-asymmetric salts at low reduced temperatures. *J. Mol. Liquids*, 131–132:179–184, 2007. IF: 0.982. #Refs = 12.
- [67] D. Di Caprio, M. Valiskó, M. Holovko, and D. Boda. Anomalous temperature dependence of the differential capacitance in valence asymmetric electrolytes. Comparison of Monte Carlo simulation results and the field theoretical approach. *Mol. Phys.*, 104(22-24):3777–3786, 2006. IF: 1.690. #Refs = 10.
- [68] A. Malasics, D. Boda, and M. Valiskó. Monte Carlo simulation and renormalized perturbation theory study of the dielectric properties of mixtures of polarizable hard spheres and polarizable dipolar hard spheres. *Mol. Phys.*, 104(22-24):3821–3830, 2006. IF: 1.690. #Refs = 1.
- [69] D. Boda, M. Valiskó, B. Eisenberg, W. Nonner, D. Henderson, and D. Gillespie. The effect of protein dielectric coefficient on the ionic selectivity of a calcium channel. *J. Chem. Phys.*, 125(3):034901, 2006. IF: 3.166. #Refs = 30.
- [70] D. Boda, D. Gillespie, B. Eisenberg, W. Nonner, and D. Henderson. *Ionic Soft Matter: Novel Trends in Theory and Applications*, volume 206 of *NATO Science Series: II: Mathematics, Physics and Chemistry*, chapter The Induced Charge Computation Method and its Application in Monte Carlo Simulations of Inhomogeneous Dielectric Systems, pages 19–44. Springer, Dordrecht, The Netherlands, 2005. #Refs = 1.
- [71] D. Gillespie, M. Valiskó, and D. Boda. Density functional theory of the electrical double layer: the RFD functional. *J. Phys.-Cond. Matt.*, 17(42):6609–6626, 2005. IF: 2.145. #Refs = 67.
- [72] D. Henderson, D. Gillespie, T. Nagy, and D. Boda. Monte Carlo simulation of the electric double layer: Dielectric boundaries and the effects of induced charge. *Mol. Phys.*, 103(21-23):2851–2861, 2005. IF: 1.351. #Refs = 24.
- [73] M. Valiskó and D. Boda. Dielectric constant of the polarizable dipolar hard sphere fluid studied by Monte Carlo simulation and theories. *Condensed Matter Phys.*, 8(2):357–376, 2005. IF: 0.621. #Refs = 12.
- [74] D. Henderson and D. Boda. On a conjecture of Fawcett. *J. Electroanalytical Chem.*, 582(1-2):16–20, 2005. IF: 2.223. #Refs = 7.
- [75] M. Valiskó and D. Boda. Relative permittivity of polar liquids. Comparison of theory, experiment, and simulation. *J. Phys. Chem. B*, 109(13):6355–6365, 2005. IF: 4.033. #Refs = 15.
- [76] J. Reszko-Zygmunt, S. Sokołowski, D. Henderson, and D. Boda. Temperature dependence of the double layer capacitance for the restricted primitive model of an electrolyte solution from a density functional approach. *J. Chem. Phys.*, 122(8):084504, 2005. IF: 3.138. #Refs = 51.

- [77] D. Boda, D. Gillespie, W. Nonner, D. Henderson, D. Busath, and B. Eisenberg. Effects of dielectrics on selectivity: Computing induced charge in Monte Carlo simulations. *Biophys. J.*, 86(1):6A–6A, 2004. #Refs = 1.
- [78] M. Valiskó, D. Henderson, and D. Boda. Competition between the effects of asymmetries in ion diameters and charges in an electrical double layer studied by Monte Carlo simulations and theories. *J. Phys. Chem. B*, 108(42):16548–16555, 2004. IF: 3.834. #Refs = 54.
- [79] D. Boda, D. Gillespie, W. Nonner, D. Henderson, and B. Eisenberg. Computing induced charges in inhomogeneous dielectric media: Application in a Monte Carlo simulation of complex ionic systems. *Phys. Rev. E*, 69(4):046702, 2004. IF: 2.352. #Refs = 77.
- [80] T. Kristóf, D. Boda, and D. Henderson. Phase separation in mixtures of Yukawa and charged Yukawa particles from Gibbs ensemble Monte Carlo simulations and the mean spherical approximation. *J. Chem. Phys.*, 120(6):2846–2850, 2004. IF: 3.105. #Refs = 3.
- [81] D. Boda, T. Varga, D. Henderson, D. D. Busath, W. Nonner, D. Gillespie, and B. Eisenberg. Monte Carlo simulation study of a system with a dielectric boundary: Application to calcium channel selectivity. *Mol. Simulation*, 30(2-3):89–96, 2004. IF: 1.241. #Refs = 12.
- [82] D. Boda, D. Henderson, P. Plaschko, and W. R. Fawcett. Monte Carlo and density functional theory study of the electrical double layer: The dependence of the charge/voltage relation on the diameter of the ions. *Mol. Simulation*, 30(2-3):137–141, 2004. IF: 1.241. #Refs = 27.
- [83] M. Valiskó, D. Boda, J. Liszi, and I. Szalai. A systematic Monte Carlo simulation and renormalized perturbation theoretical study of the dielectric constant of the polarizable Stockmayer fluid. *Mol. Phys.*, 101(14):2309–2313, 2003. IF: 1.591. #Refs = 6.
- [84] T. Kristóf, D. Boda, J. Liszi, D. Henderson, and E. Carlson. Vapour-liquid equilibrium of the charged Yukawa fluid from Gibbs ensemble Monte Carlo simulations and the mean spherical approximation. *Mol. Phys.*, 101(11):1611–1616, 2003. IF: 1.591. #Refs = 14.
- [85] Y. Yang, D. Boda, D. Henderson, and D. D. Busath. Computer simulation studies of the selectivity and conductance of a model calcium channel. *J. Comp. Electronics*, 1(3):353–357, 2002. IF: -.
- [86] D. Boda, D. Henderson, L. M. Y. Teran, and S. Sokołowski. The application of density functional theory and the generalized mean spherical approximation to double layers containing strongly coupled ions. *J. Physics-condensed Matter*, 14(46):11945–11954, 2002. IF: 1.775. #Refs = 18.
- [87] D. Boda and D. Henderson. Computer simulation of the selectivity of a model calcium channel. *J. Physics-condensed Matter*, 14(41):9485–9488, 2002. IF: 1.775. #Refs = 2.
- [88] D. Boda, D. D. Busath, B. Eisenberg, D. Henderson, and W. Nonner. Monte Carlo simulations of ion selectivity in a biological Na channel: Charge-space competition. *Phys. Chem. Chem. Phys.*, 4(20):5154–5160, 2002. IF: 1.838. #Refs = 28.
- [89] T. Kristóf, J. Liszi, and D. Boda. The extrapolation of phase equilibrium curves of mixtures in the isobaric-isothermal Gibbs ensemble. *Mol. Phys.*, 100(21):3429–3441, 2002. IF: 1.617. #Refs = 7.
- [90] M. Valiskó, D. Boda, J. Liszi, and I. Szalai. The dielectric constant of polarizable fluids from the renormalized perturbation theory. *Mol. Phys.*, 100(20):3239–3243, 2002. IF: 1.617. #Refs = 5.
- [91] D. Boda, D. D. Busath, and D. Henderson. Simulation of the selectivity of a calcium channel. *Appl. Surf. Science*, 196(1-4):154–156, 2002. IF: 1.295. #Refs = 1.
- [92] D. Boda, D. Henderson, and D. D. Busath. Monte Carlo study of the selectivity of calcium channels: improved geometrical model. *Mol. Phys.*, 100(14):2361–2368, 2002. IF: 1.617. #Refs = 19.

- [93] D. Boda, T. Kristóf, J. Liszi, and I. Szalai. The extrapolation of the vapour-liquid equilibrium curves of pure fluids in the isothermal Gibbs ensemble. *Mol. Phys.*, 100(12):1989–2000, 2002. IF: 1.617. #Refs = 4.
- [94] D. Boda, W. R. Fawcett, D. Henderson, and S. Sokołowski. Monte Carlo, density functional theory, and Poisson-Boltzmann theory study of the structure of an electrolyte near an electrode. *J. Chem. Phys.*, 116(16):7170–7176, 2002. IF: 2.998. #Refs = 103.
- [95] D. Boda, D. Henderson, and D. D. Busath. Monte Carlo study of the effect of ion and channel size on the selectivity of a model calcium channel. *J. Phys. Chem. B*, 105(47):11574–11577, 2001. IF: 3.379. #Refs = 34.
- [96] D. Boda, T. Kristóf, J. Liszi, and I. Szalai. A new simulation method for the determination of phase equilibria in mixtures in the grand canonical ensemble. *Mol. Phys.*, 99(24):2011–2022, 2001. IF: 1.735. #Refs = 11.
- [97] M. Valiskó, D. Boda, J. Liszi, and I. Szalai. Relative permittivity of dipolar liquids and their mixtures. Comparison of theory and experiment. *Phys. Chem. Chem. Phys.*, 3(15):2995–3000, 2001. IF: 1.787. #Refs = 15.
- [98] L. Mier-Y-Teran, D. Boda, D. Henderson, and S. E. Quinones-Cisneros. On the low temperature anomalies in the properties of the electrochemical interface. A non-local free-energy density functional approach. *Mol. Phys.*, 99(15):1323–1328, 2001. IF: 1.735. #Refs = 7.
- [99] D. Boda, D. Henderson, A. Patrykiewicz, and S. Sokołowski. Density functional study of a simple membrane using the solvent primitive model. *J. Colloid Interface Science*, 239(2):432–439, 2001. IF: 1.530. #Refs = 6.
- [100] M. Holovko, V. Kapko, D. Henderson, and D. Boda. On the influence of ionic association on the capacitance of an electrical double layer. *Chem. Phys. Lett.*, 341(3-4):363–368, 2001. IF: 2.364. #Refs = 52.
- [101] T. Kristóf, D. Boda, I. Szalai, and D. Henderson. A Gibbs ensemble Monte Carlo study of phase coexistence in the solvent primitive model. *J. Chem. Phys.*, 113(17):7488–7491, 2000. IF: 3.301. #Refs = 10.
- [102] B. V. R. Tata, D. Boda, D. Henderson, A. Nikolov, and D. T. Wasan. Structure of charged colloids under a wedge confinement. *Phys. Rev. E*, 62(3):3875–3881, 2000. IF: 2.142. #Refs = 21.
- [103] D. Boda, D. D. Busath, D. Henderson, and S. Sokołowski. Monte Carlo simulations of the mechanism for channel selectivity: The competition between volume exclusion and charge neutrality. *J. Phys. Chem. B*, 104(37):8903–8910, 2000. IF: 3.386. #Refs = 64.
- [104] D. Henderson, D. Boda, and D. T. Wasan. A generalized mean spherical approximation of the anomalies in the electrochemical double layer for strong ionic interactions. *Chem. Phys. Lett.*, 325(5-6):655–660, 2000. IF: 2.364. #Refs = 7.
- [105] P. S. Crozier, R. L. Rowley, D. Henderson, and D. Boda. A corrected 3D Ewald calculation of the low effective temperature properties of the electrochemical interface. *Chem. Phys. Lett.*, 325(5-6):675–677, 2000. IF: 2.368. #Refs = 8.
- [106] S. Varga, D. Boda, D. Henderson, and S. Sokołowski. Density functional theory and the capillary evaporation of a liquid in a slit. *J. Colloid Interface Science*, 227(1):223–226, 2000. IF: 1.494. #Refs = 25.

- [107] D. Boda, D. Henderson, A. Patrykiewicz, and S. Sokołowski. Simulation and density functional study of a simple membrane. II. Solvent effects using the solvent primitive model. *J. Chem. Phys.*, 113(2):802–806, 2000. IF: 3.301. #Refs = 15.
- [108] D. Boda and D. Henderson. The capacitance of the solvent primitive model double layer at low effective temperatures. *J. Chem. Phys.*, 112(20):8934–8938, 2000. IF: 3.301. #Refs = 27.
- [109] P. Bryk, A. Patrykiewicz, S. Sololowski, D. Boda, and D. Henderson. Ions at membranes: a density functional approach. *Phys. Chem. Chem. Phys.*, 2(2):269–276, 2000. IF: 1.653. #Refs = 1.
- [110] D. Boda and D. Henderson. Theory and simulation of the electrical double layer. In *Annales Universitatis Mariae Curie-Skłodowska*, volume 54-55 of *Sectio AA Chemia*, pages 171–186. Lublin, Polonia, 1999.
- [111] D. Boda, D. Henderson, R. Rowley, and S. Sokołowski. Simulation and density functional study of a simple membrane separating two restricted primitive model electrolytes. *J. Chem. Phys.*, 111(20):9382–9388, 1999. IF: 3.289. #Refs = 24.
- [112] D. Boda, D. Henderson, K. Y. Chan, and D. T. Wasan. Low temperature anomalies in the properties of the electrochemical interface. *Chem. Phys. Lett.*, 308(5-6):473–478, 1999. IF: 2.269. #Refs = 41.
- [113] D. Boda, K. Y. Chan, D. Henderson, D. T. Wasan, and A. D. Nikolov. Structure and pressure of a hard sphere fluid in a wedge-shaped cell or meniscus. *Langmuir*, 15(13):4311–4313, 1999. IF: 2.937. #Refs = 16.
- [114] I. Szalai, D. Henderson, D. Boda, and K. Y. Chan. Thermodynamics and structural properties of the dipolar Yukawa fluid. *J. Chem. Phys.*, 111(1):337–344, 1999. IF: 3.289. #Refs = 22.
- [115] D. Henderson, D. Boda, I. Szalai, and K. Y. Chan. The mean spherical approximation for a dipolar Yukawa fluid. *J. Chem. Phys.*, 110(15):7348–7353, 1999. IF: 3.289. #Refs = 21.
- [116] D. Boda, D. Henderson, and K. Y. Chan. Monte Carlo study of the capacitance of the double layer in a model molten salt. *J. Chem. Phys.*, 110(11):5346–5350, 1999. IF: 3.289. #Refs = 85.
- [117] D. Henderson, D. Boda, K. Y. Chan, and D. T. Wasan. Phase separation in fluid additive hard sphere mixtures? *Mol. Phys.*, 95(2):131–135, 1998. IF: 1.854. #Refs = 20.
- [118] D. Boda, K. Y. Chan, and D. Henderson. Monte Carlo simulation of an ion-dipole mixture as a model of an electrical double layer. *J. Chem. Phys.*, 109(17):7362–7371, 1998. IF: 3.147. #Refs = 92.
- [119] D. Boda, K. Y. Chan, and I. Szalai. Determination of vapour-liquid equilibrium using cavity-biased grand canonical Monte Carlo method. *Mol. Phys.*, 92(6):1067–1072, 1997. IF: 1.700. #Refs = 14.
- [120] D. Boda, J. Liszi, and I. Szalai. The extended NpT and NVT plus test particle methods for the determination of vapour-liquid equilibria of pure fluids. *Magyar Kémiai Folyóirat*, 102(12):523–534, 1996. IF: 0.107.
- [121] D. Boda, T. Lukács, J. Liszi, and I. Szalai. The isochoric-, isobaric- and saturation-heat capacities of the Lennard-Jones fluid from equations of state and Monte Carlo simulations. *Fluid Phase Equilibria*, 119(1-2):1–16, 1996. IF: 1.153. #Refs = 12.
- [122] D. Boda, B. Kalmár, J. Liszi, and I. Szalai. Fluid-fluid equilibrium of a mixture of non-polar and dipolar hard spheres in an applied field. *J. Chem. Society-Faraday Transactions*, 92(15):2709–2714, 1996. IF: 1.663. #Refs = 3.
- [123] D. Boda, J. Liszi, and I. Szalai. A new simulation method for the determination of the vapour-liquid equilibria in the grand canonical ensemble. *Chem. Phys. Lett.*, 256(4-5):474–482, 1996. IF: 2.589. #Refs = 11.

- [124] D. Boda, J. C. Winkelmann, J. Liszi, and I. Szalai. Vapour-liquid equilibrium of Stockmayer fluids in applied field - Application of the NpTE plus test particle method and perturbation theory. *Mol. Phys.*, 87(3):601–624, 1996. IF: 1.581. #Refs = 27.
- [125] I. Szalai, J. Liszi, and D. Boda. The NVT plus test particle method for the determination of the vapor-liquid-equilibria of pure fluids. *Chem. Phys. Lett.*, 246(3):214–220, 1995. IF: 2.509. #Refs = 15.
- [126] D. Boda, J. Liszi, and I. Szalai. Preliminary communication - dielectric-constant of a Stockmayer fluid along the vapor-liquid coexistence curve. *Mol. Phys.*, 85(3):429–434, 1995. IF: 1.827. #Refs = 13.
- [127] D. Boda, J. Liszi, and I. Szalai. An extension of the NpT plus test particle method for the determination of the vapor-liquid-equilibria of pure fluids. *Chem. Phys. Lett.*, 235(1-2):140–145, 1995. IF: 2.509. #Refs = 23.
- [128] D. Boda, I. Szalai, and J. Liszi. Influence of static electric-field on the vapor-liquid coexistence of dipolar soft-sphere fluids. *J. Chem. Society-faraday Transactions*, 91(5):889–894, 1995. IF: 1.771. #Refs = 12.
- [129] J. Liszi, D. Boda, and I. Szalai. Perturbation theoretical results of thermodynamic and dielectric studies on polar fluids. *ACH-Models in Chem.*, 132(1-2):31–43, 1995. IF: 0.390. #Refs = 1.