



UvA-DARE (Digital Academic Repository)

Self-assembly via anisotropic interactions

Modeling association kinetics of patchy particle systems and self-assembly induced by critical Casimir forces

Newton, A.C.

Publication date

2017

Document Version

Other version

License

Other

[Link to publication](#)

Citation for published version (APA):

Newton, A. C. (2017). *Self-assembly via anisotropic interactions: Modeling association kinetics of patchy particle systems and self-assembly induced by critical Casimir forces*. [Thesis, fully internal, Universiteit van Amsterdam].

General rights

It is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), other than for strictly personal, individual use, unless the work is under an open content license (like Creative Commons).

Disclaimer/Complaints regulations

If you believe that digital publication of certain material infringes any of your rights or (privacy) interests, please let the Library know, stating your reasons. In case of a legitimate complaint, the Library will make the material inaccessible and/or remove it from the website. Please Ask the Library: <https://uba.uva.nl/en/contact>, or a letter to: Library of the University of Amsterdam, Secretariat, Singel 425, 1012 WP Amsterdam, The Netherlands. You will be contacted as soon as possible.

References

- [1] G. M. Whitesides and M. Boncheva, “Beyond molecules: Self-assembly of mesoscopic and macroscopic components,” *Proceedings of the National Academy of Sciences*, vol. 99, no. 8, pp. 4769–4774, 2002.
- [2] J. Halley, D. A. Winkler, *et al.*, “Consistent concepts of self-organization and self-assembly,” *Complexity*, vol. 14, no. 2, pp. 10–17, 2008.
- [3] J. A. Luiken and P. G. Bolhuis, “Prediction of a stable associated liquid of short amyloidogenic peptides,” *Physical Chemistry Chemical Physics*, vol. 17, no. 16, pp. 10556–10567, 2015.
- [4] Q. Chen, S. C. Bae, and S. Granick, “Directed self-assembly of a colloidal kagome lattice,” *Nature*, vol. 469, no. 7330, pp. 381–384, 2011.
- [5] D. J. Kraft, R. Ni, F. Smalenburg, M. Hermes, K. Yoon, D. A. Weitz, A. van Blaaderen, J. Groenewold, M. Dijkstra, and W. K. Kegel, “Surface roughness directed self-assembly of patchy particles into colloidal micelles,” *Proceedings of the National Academy of Sciences*, vol. 109, no. 27, pp. 10787–10792, 2012.
- [6] J. R. Wolters, G. Avvisati, F. Hagemans, T. Vissers, D. J. Kraft, M. Dijkstra, and W. K. Kegel, “Self-assembly of Mickey Mouse shaped colloids into tube-like structures: experiments and simulations,” *Soft Matter*, vol. 11, no. 6, pp. 1067–1077, 2015.
- [7] D. L. Caspar and A. Klug, “Physical principles in the construction of regular viruses,” in *Cold Spring Harbor symposia on quantitative biology*, vol. 27, pp. 1–24, Cold Spring Harbor Laboratory Press, 1962.
- [8] A. Klug and D. L. Caspar, “The structure of small viruses,” *Advances in virus research*, vol. 7, pp. 225–325, 1961.
- [9] F. Crick and J. Watson, “Virus structure: general principles,” in *The Nature of Viruses*, pp. 5–18, Churchill London, 1957.
- [10] E. J. Corey, *The logic of chemical synthesis*. John Wiley and Sons, 1989.
- [11] E. Corey, “Robert robinson lecture. retrosynthetic thinking: essentials and examples,” *Chemical Society Reviews*, vol. 17, pp. 111–133, 1988.

-
- [12] F. Aricó, J. D. Badjic, S. J. Cantrill, A. H. Flood, K. C.-F. Leung, Y. Liu, and J. F. Stoddart, “Templated synthesis of interlocked molecules,” in *Templates in Chemistry II*, pp. 203–259, Springer, 2005.
- [13] S. C. Glotzer and M. J. Solomon, “Anisotropy of building blocks and their assembly into complex structures,” *Nature materials*, vol. 6, no. 8, pp. 557–562, 2007.
- [14] S. Sacanna and D. J. Pine, “Shape-anisotropic colloids: Building blocks for complex assemblies,” *Current Opinion in Colloid & Interface Science*, vol. 16, no. 2, pp. 96–105, 2011.
- [15] A. A. Shah, B. Schultz, K. L. Kohlstedt, S. C. Glotzer, and M. J. Solomon, “Synthesis, assembly, and image analysis of spheroidal patchy particles,” *Langmuir*, vol. 29, no. 15, pp. 4688–4696, 2013.
- [16] Y. Wang, Y. Wang, D. R. Breed, V. N. Manoharan, L. Feng, A. D. Hollingsworth, M. Weck, and D. J. Pine, “Colloids with valence and specific directional bonding,” *Nature*, vol. 491, no. 7422, pp. 51–55, 2012.
- [17] Q. Chen, J. K. Whitmer, S. Jiang, S. C. Bae, E. Luijten, and S. Granick, “Supracolloidal reaction kinetics of janus spheres,” *Science*, vol. 331, no. 6014, pp. 199–202, 2011.
- [18] S. Sacanna, W. Irvine, P. M. Chaikin, and D. J. Pine, “Lock and key colloids,” *Nature*, vol. 464, no. 7288, pp. 575–578, 2010.
- [19] C. H. Evers, J. A. Luiken, P. G. Bolhuis, and W. K. Kegel, “Self-assembly of microcapsules via colloidal bond hybridization and anisotropy,” *Nature*, 2016.
- [20] X. Mao, Q. Chen, and S. Granick, “Entropy favours open colloidal lattices,” *Nature materials*, vol. 12, no. 3, pp. 217–222, 2013.
- [21] S. Whitelam, “Control of pathways and yields of protein crystallization through the interplay of nonspecific and specific attractions,” *Physical review letters*, vol. 105, no. 8, p. 088102, 2010.
- [22] V. Meester, R. W. Verweij, C. van der Wel, and D. J. Kraft, “Colloidal recycling: Reconfiguration of random aggregates into patchy particles,” *ACS nano*, vol. 10, no. 4, pp. 4322–4329, 2016.
- [23] G. van Anders, N. K. Ahmed, R. Smith, M. Engel, and S. C. Glotzer, “Entropically patchy particles: Engineering valence through shape entropy,” *ACS nano*, vol. 8, no. 1, pp. 931–940, 2013.
- [24] J. Yan, K. Chaudhary, S. C. Bae, J. A. Lewis, and S. Granick, “Colloidal ribbons and rings from janus magnetic rods,” *Nature communications*, vol. 4, p. 1516, 2013.

-
- [25] W. Liu, M. Tagawa, H. L. Xin, T. Wang, H. Emamy, H. Li, K. G. Yager, F. W. Starr, A. V. Tkachenko, and O. Gang, “Diamond family of nanoparticle superlattices,” *Science*, vol. 351, no. 6273, pp. 582–586, 2016.
- [26] A. Yethiraj and A. van Blaaderen, “A colloidal model system with an interaction tunable from hard sphere to soft and dipolar,” *Nature*, vol. 421, no. 6922, pp. 513–517, 2003.
- [27] M. Krech, *The Casimir effect in critical systems*. World Scientific, 1994.
- [28] C. Hertlein, L. Helden, A. Gambassi, S. Dietrich, and C. Bechinger, “Direct measurement of critical casimir forces,” *Nature*, vol. 451, no. 7175, pp. 172–175, 2008.
- [29] A. Gambassi, *The Casimir effect: From quantum to critical fluctuations*, vol. 161. IOP Publishing, 2009.
- [30] A. Gambassi, A. Maciołek, C. Hertlein, U. Nellen, L. Helden, C. Bechinger, and S. Dietrich, “Critical casimir effect in classical binary liquid mixtures,” *Physical Review E*, vol. 80, no. 6, p. 061143, 2009.
- [31] U. Nellen, J. Dietrich, L. Helden, S. Chodankar, K. Nygård, J. F. van der Veen, and C. Bechinger, “Salt-induced changes of colloidal interactions in critical mixtures,” *Soft Matter*, vol. 7, no. 11, pp. 5360–5364, 2011.
- [32] M. E. Fisher and P. G. de Gennes, “Wall phenomena in a critical binary mixture,” *Comptes Rendus Hebdomadaires Des Seances De L Academie Des Sciences Serie B*, vol. 287, no. 8, pp. 207–209, 1978.
- [33] H. Guo, T. Narayanan, M. Sztuchi, P. Schall, and G. H. Wegdam, “Reversible phase transition of colloids in a binary liquid solvent,” *Physical review letters*, vol. 100, no. 18, p. 188303, 2008.
- [34] M. T. Dang, A. V. Verde, P. G. Bolhuis, P. Schall, *et al.*, “Temperature-sensitive colloidal phase behavior induced by critical casimir forces,” *The Journal of chemical physics*, vol. 139, no. 9, p. 094903, 2013.
- [35] D. Bonn, J. Otwinowski, S. Sacanna, H. Guo, G. Wegdam, and P. Schall, “Direct observation of colloidal aggregation by critical casimir forces,” *Physical review letters*, vol. 103, no. 15, p. 156101, 2009.
- [36] S. Faber, Z. Hu, G. H. Wegdam, P. Schall, *et al.*, “Controlling colloidal phase transitions with critical casimir forces,” *Nature communications*, vol. 4, p. 1584, 2013.
- [37] V. Nguyen, M. Dang, T. Nguyen, and P. Schall, “Critical casimir forces for colloidal assembly,” *Journal of Physics: Condensed Matter*, vol. 28, no. 4, p. 043001, 2016.

-
- [38] J. R. Edison, N. Tasios, S. Belli, R. Evans, R. van Roij, and M. Dijkstra, “Critical casimir forces and colloidal phase transitions in a near-critical solvent: A simple model reveals a rich phase diagram,” *Physical review letters*, vol. 114, no. 3, p. 038301, 2015.
- [39] N. Tasios, J. R. Edison, R. van Roij, R. Evans, and M. Dijkstra, “Critical casimir interactions and colloidal self-assembly in near-critical solvents,” *The Journal of Chemical Physics*, vol. 145, no. 8, p. 084902, 2016.
- [40] T. Mohry, A. Maciołek, and S. Dietrich, “Phase behavior of colloidal suspensions with critical solvents in terms of effective interactions,” *The Journal of chemical physics*, vol. 136, no. 22, p. 224902, 2012.
- [41] S. Buzzaccaro, J. Colombo, A. Parola, and R. Piazza, “Critical depletion,” *Physical review letters*, vol. 105, no. 19, p. 198301, 2010.
- [42] A. Hanke, F. Schlesener, E. Eisenriegler, and S. Dietrich, “Critical casimir forces between spherical particles in fluids,” *Physical review letters*, vol. 81, no. 9, p. 1885, 1998.
- [43] O. Vasilyev, A. Gambassi, A. Maciołek, and S. Dietrich, “Universal scaling functions of critical casimir forces obtained by monte carlo simulations,” *Physical Review E*, vol. 79, no. 4, p. 041142, 2009.
- [44] O. Vasilyev, A. Gambassi, A. Maciołek, and S. Dietrich, “Monte carlo simulation results for critical casimir forces,” *EPL (Europhysics Letters)*, vol. 80, no. 6, p. 60009, 2007.
- [45] F. Schlesener, A. Hanke, and S. Dietrich, “Critical casimir forces in colloidal suspensions,” *Journal of statistical physics*, vol. 110, no. 3-6, pp. 981–1013, 2003.
- [46] T. Mohry, S. Kondrat, A. Maciołek, and S. Dietrich, “Critical casimir interactions around the consolute point of a binary solvent,” *Soft matter*, vol. 10, no. 30, pp. 5510–5522, 2014.
- [47] T. Mohry, A. Maciołek, and S. Dietrich, “Structure and aggregation of colloids immersed in critical solvents,” *The Journal of chemical physics*, vol. 136, no. 22, p. 224903, 2012.
- [48] D. Frenkel and B. Smit, “Understanding molecular simulations: from algorithms to applications,” *Academic, San Diego*, 1996.
- [49] E. Verwey and J. T. G. Overbeek, “Theory of the stability of lyophobic colloids,” *Journal of Colloid Science*, vol. 10, no. 2, pp. 224–225, 1955.
- [50] M. G. Noro and D. Frenkel, “Extended corresponding-states behavior for particles with variable range attractions,” *The Journal of Chemical Physics*, vol. 113, no. 8, pp. 2941–2944, 2000.

-
- [51] G. Foffi and F. Sciortino, “On the possibility of extending the noro-frenkel generalized law of correspondent states to nonisotropic patchy interactions,” *The Journal of Physical Chemistry B*, vol. 111, no. 33, pp. 9702–9705, 2007.
- [52] N. Kern and D. Frenkel, “Fluid–fluid coexistence in colloidal systems with short-ranged strongly directional attraction,” *The Journal of chemical physics*, vol. 118, no. 21, pp. 9882–9889, 2003.
- [53] F. Romano, E. Sanz, and F. Sciortino, “Phase diagram of a tetrahedral patchy particle model for different interaction ranges,” *The Journal of Chemical Physics*, vol. 132, no. 18, p. 184501, 2010.
- [54] F. Romano and F. Sciortino, “Colloidal self-assembly: patchy from the bottom up,” *Nature materials*, vol. 10, no. 3, pp. 171–173, 2011.
- [55] F. Smallenburg and F. Sciortino, “Liquids more stable than crystals in particles with limited valence and flexible bonds,” *Nature Physics*, vol. 9, no. 9, pp. 554–558, 2013.
- [56] F. Romano and F. Sciortino, “Patterning symmetry in the rational design of colloidal crystals,” *Nature communications*, vol. 3, p. 975, 2012.
- [57] G. Munao, Z. Preisler, T. Vissers, F. Smallenburg, and F. Sciortino, “Cluster formation in one-patch colloids: low coverage results,” *Soft Matter*, vol. 9, no. 9, pp. 2652–2661, 2013.
- [58] T. Vissers, Z. Preisler, F. Smallenburg, M. Dijkstra, and F. Sciortino, “Predicting crystals of janus colloids,” *The Journal of chemical physics*, vol. 138, no. 16, p. 164505, 2013.
- [59] Z. Preisler, T. Vissers, G. Munao, F. Smallenburg, and F. Sciortino, “Equilibrium phases of one-patch colloids with short-range attractions,” *Soft Matter*, vol. 10, no. 28, pp. 5121–5128, 2014.
- [60] T. Vissers, F. Smallenburg, G. Munao, Z. Preisler, and F. Sciortino, “Cooperative polymerization of one-patch colloids,” *The Journal of chemical physics*, vol. 140, no. 14, p. 144902, 2014.
- [61] A. W. Wilber, J. P. Doye, A. A. Louis, E. G. Noya, M. A. Miller, and P. Wong, “Reversible self-assembly of patchy particles into monodisperse icosahedral clusters,” *The Journal of chemical physics*, vol. 127, no. 8, p. 085106, 2007.
- [62] J. P. Doye, A. A. Louis, I.-C. Lin, L. R. Allen, E. G. Noya, A. W. Wilber, H. C. Kok, and R. Lyus, “Controlling crystallization and its absence: proteins, colloids and patchy models,” *Physical Chemistry Chemical Physics*, vol. 9, no. 18, pp. 2197–2205, 2007.

-
- [63] A. W. Wilber, J. P. Doye, and A. A. Louis, “Self-assembly of monodisperse clusters: Dependence on target geometry,” *The Journal of chemical physics*, vol. 131, no. 17, p. 175101, 2009.
- [64] R. Guo, J. Mao, X.-M. Xie, and L.-T. Yan, “Predictive supracolloidal helices from patchy particles,” *Scientific reports*, vol. 4, 2014.
- [65] G. Avvisati, T. Vissers, and M. Dijkstra, “Self-assembly of patchy colloidal dumbbells,” *The Journal of chemical physics*, vol. 142, no. 8, p. 084905, 2015.
- [66] Z. Zhang and S. C. Glotzer, “Self-assembly of patchy particles,” *Nano Letters*, vol. 4, no. 8, pp. 1407–1413, 2004.
- [67] A. Vijaykumar, P. G. Bolhuis, and P. R. ten Wolde, “The intrinsic rate constants in diffusion-influenced reactions,” *Faraday Discussions*, 2016.
- [68] F. Smallenburg, L. Filion, and F. Sciortino, “Erasing no-man’s land by thermodynamically stabilizing the liquid-liquid transition in tetrahedral particles,” *Nature physics*, vol. 10, no. 9, pp. 653–657, 2014.
- [69] Z. Zhang, A. S. Keys, T. Chen, and S. C. Glotzer, “Self-assembly of patchy particles into diamond structures through molecular mimicry,” *Langmuir*, vol. 21, no. 25, pp. 11547–11551, 2005.
- [70] M. F. Hagan and D. Chandler, “Dynamic pathways for viral capsid assembly,” *Biophysical journal*, vol. 91, no. 1, pp. 42–54, 2006.
- [71] M. R. Perkett and M. F. Hagan, “Using markov state models to study self-assembly,” *The Journal of chemical physics*, vol. 140, no. 21, p. 214101, 2014.
- [72] S. Whitelam and R. L. Jack, “The statistical mechanics of dynamic pathways to self-assembly,” *arXiv preprint arXiv:1407.2505*, 2014.
- [73] S. Whitelam, E. H. Feng, M. F. Hagan, and P. L. Geissler, “The role of collective motion in examples of coarsening and self-assembly,” *Soft Matter*, vol. 5, no. 6, pp. 1251–1262, 2009.
- [74] S. Whitelam and P. L. Geissler, “Avoiding unphysical kinetic traps in monte carlo simulations of strongly attractive particles,” *The Journal of chemical physics*, vol. 127, no. 15, p. 154101, 2007.
- [75] K. Takahashi, S. Tănase-Nicola, and P. R. Ten Wolde, “Spatio-temporal correlations can drastically change the response of a mapk pathway,” *Proceedings of the National Academy of Sciences*, vol. 107, no. 6, pp. 2473–2478, 2010.
- [76] A. D. Fokker, “Die mittlere energie rotierender elektrischer dipole im strahlungsfeld,” *Annalen der Physik*, vol. 348, no. 5, pp. 810–820, 1914.

-
- [77] M. Planck, *Über einen Satz der Statistischen Dynamik und seine Erweiterung in der Quantentheorie*. Reimer, 1917.
- [78] M. v. Smoluchowski, "Grundriß der koagulationskinetik kolloider lösungen," *Colloid & Polymer Science*, vol. 21, no. 3, pp. 98–104, 1917.
- [79] M. Smoluchowski, "Versuch einer mathematischen theorie der koagulation-skinetik kolloider lösungen," *Pisma Mariana Smoluchowskiego*, vol. 2, no. 1, pp. 595–639, 1927.
- [80] A. Kolmogoroff, "Über die analytischen methoden in der wahrscheinlichkeit-srechnung," *Mathematische Annalen*, vol. 104, no. 1, pp. 415–458, 1931.
- [81] F. C. Collins and G. E. Kimball, "Diffusion-controlled reaction rates," *Journal of colloid science*, vol. 4, no. 4, pp. 425–437, 1949.
- [82] N. Van Kampen, "Derivation of the phenomenological equations from the master equation: I. even variables only," *Physica*, vol. 23, no. 6-10, pp. 707–719, 1957.
- [83] S. H. Northrup and H. P. Erickson, "Kinetics of protein-protein association explained by brownian dynamics computer simulation.," *Proceedings of the National Academy of Sciences*, vol. 89, no. 8, pp. 3338–3342, 1992.
- [84] D. Shoup and A. Szabo, "Role of diffusion in ligand binding to macromolecules and cell-bound receptors.," *Biophysical Journal*, vol. 40, no. 1, p. 33, 1982.
- [85] A. Szabo, K. Schulten, and Z. Schulten, "First passage time approach to diffusion controlled reactions," *The Journal of chemical physics*, vol. 72, no. 8, pp. 4350–4357, 1980.
- [86] N. Agmon and A. Szabo, "Theory of reversible diffusion-influenced reactions," *The Journal of Chemical Physics*, vol. 92, no. 9, pp. 5270–5284, 1990.
- [87] N. G. Van Kampen, *Stochastic processes in physics and chemistry*, vol. 1. Elsevier, 1992.
- [88] P. G. Bolhuis, D. Chandler, C. Dellago, and P. L. Geissler, "Transition path sampling: Throwing ropes over rough mountain passes, in the dark," *Annual review of physical chemistry*, vol. 53, no. 1, pp. 291–318, 2002.
- [89] C. Dellago and P. G. Bolhuis, "Transition path sampling and other advanced simulation techniques for rare events," *Advances in Polymer Science*, 2008.
- [90] A. Bhattacharyay and A. Troisi, "Self-assembly of sparsely distributed molecules: An efficient cluster algorithm," *Chemical Physics Letters*, vol. 458, no. 1, pp. 210–213, 2008.

-
- [91] I. M. Ilie, W. J. Briels, and W. K. den Otter, “An elementary singularity-free rotational brownian dynamics algorithm for anisotropic particles,” *The Journal of chemical physics*, vol. 142, no. 11, p. 114103, 2015.
- [92] M. P. Allen and G. Germano, “Expressions for forces and torques in molecular simulations using rigid bodies,” *Molecular Physics*, vol. 104, no. 20-21, pp. 3225–3235, 2006.
- [93] S. Whitelam, “Approximating the dynamical evolution of systems of strongly interacting overdamped particles,” *Molecular Simulation*, vol. 37, no. 7, pp. 606–612, 2011.
- [94] F. Romano, C. De Michele, D. Marenduzzo, and E. Sanz, “Monte carlo and event-driven dynamics of brownian particles with orientational degrees of freedom,” *J. Chem. Phys.*, vol. 135, no. 12, p. 124106, 2011.
- [95] G. Vliegthart and H. N. Lekkerkerker, “Predicting the gas–liquid critical point from the second virial coefficient,” *The Journal of Chemical Physics*, vol. 112, no. 12, pp. 5364–5369, 2000.
- [96] K. V. Edmond, M. T. Elsesser, G. L. Hunter, D. J. Pine, and E. R. Weeks, “Decoupling of rotational and translational diffusion in supercooled colloidal fluids,” *Proceedings of the National Academy of Sciences*, vol. 109, no. 44, pp. 17891–17896, 2012.
- [97] C. Dellago, P. G. Bolhuis, F. S. Csajka, and D. Chandler, “Transition path sampling and the calculation of rate constants,” *The Journal of Chemical Physics*, vol. 108, no. 5, pp. 1964–1977, 1998.
- [98] C. Dellago, P. G. Bolhuis, and D. Chandler, “Efficient transition path sampling: Application to lennard-jones cluster rearrangements,” *The Journal of chemical physics*, vol. 108, no. 22, pp. 9236–9245, 1998.
- [99] P. G. Bolhuis, C. Dellago, and D. Chandler, “Reaction coordinates of biomolecular isomerization,” *Proceedings of the National Academy of Sciences*, vol. 97, no. 11, pp. 5877–5882, 2000.
- [100] T. S. van Erp, D. Moroni, and P. G. Bolhuis, “A novel path sampling method for the calculation of rate constants,” *Journal of Chemical Physics*, vol. 118, p. 7762, 2003.
- [101] T. S. Van Erp and P. G. Bolhuis, “Elaborating transition interface sampling methods,” *Journal of computational Physics*, vol. 205, no. 1, pp. 157–181, 2005.
- [102] T. S. van Erp, “Reaction rate calculation by parallel path swapping,” *Physical review letters*, vol. 98, no. 26, p. 268301, 2007.

-
- [103] P. G. Bolhuis, “Rare events via multiple reaction channels sampled by path replica exchange,” *The Journal of chemical physics*, vol. 129, no. 11, p. 114108, 2008.
- [104] W.-N. Du and P. G. Bolhuis, “Adaptive single replica multiple state transition interface sampling,” *The Journal of chemical physics*, vol. 139, no. 4, p. 044105, 2013.
- [105] F. Wang and D. Landau, “Efficient, multiple-range random walk algorithm to calculate the density of states,” *Physical review letters*, vol. 86, no. 10, p. 2050, 2001.
- [106] D. W. Swenson and P. G. Bolhuis, “A replica exchange transition interface sampling method with multiple interface sets for investigating networks of rare events,” *The Journal of chemical physics*, vol. 141, no. 4, p. 044101, 2014.
- [107] J. Rogal, W. Lechner, J. Juraszek, B. Ensing, and P. G. Bolhuis, “The reweighted path ensemble,” *The Journal of chemical physics*, vol. 133, no. 17, p. 174109, 2010.
- [108] W. Du and P. G. Bolhuis, “Sampling the equilibrium kinetic network of trp-cage in explicit solvent,” *The Journal of chemical physics*, vol. 140, no. 19, p. 195102, 2014.
- [109] W. E and E. Vanden-Eijnden, “Transition-Path Theory and Path-Finding Algorithms for the Study of Rare Events,” *Annual Review of Physical Chemistry*, vol. 61, pp. 391–420, 2010.
- [110] F. Noé, C. Schütte, E. Vanden-Eijnden, L. Reich, and T. R. Weikl, “Constructing the equilibrium ensemble of folding pathways from short off-equilibrium simulations,” *Proceedings of the National Academy of Sciences*, vol. 106, no. 45, pp. 19011–19016, 2009.
- [111] D. J. Kraft, J. Groenewold, and W. K. Kegel, “Colloidal molecules with well-controlled bond angles,” *Soft Matter*, vol. 5, no. 20, pp. 3823–3826, 2009.
- [112] A. Nguyen, A. C. Newton, S. J. Veen, D. Kraft, P. G. Bolhuis, and P. Schall, “Switching colloidal superstructures by critical casimir forces,” *submitted*, 2016.
- [113] B. V. Derjaguin and L. Landau, “Theory of the stability of strongly charged lyophobic sols and of the adhesion of strongly charged particles in solutions of electrolytes,” *Acta physicochim. URSS*, vol. 14, no. 6, pp. 633–662, 1941.
- [114] E. Verwey and J. T. G. Overbeek, “Theory of stability of lyophobic solids,” 1948.

-
- [115] S. Asakura and F. Oosawa, "On interaction between 2 bodies immersed in a solution of macromolecules," *J. Chem. Phys.*, vol. 22, pp. 1255–1256, 1954.
- [116] N. Kern and D. Frenkel, "Fluid-fluid coexistence in colloidal systems with short-ranged strongly directional attraction," *J. Chem. Phys.*, vol. 118, pp. 9882–9889, 2003.
- [117] D. Chandler and H. C. Andersen, "Optimized cluster expansions for classical fluids. ii. theory of molecular liquids," *The Journal of Chemical Physics*, vol. 57, no. 5, pp. 1930–1937, 1972.
- [118] L. J. Lowden and D. Chandler, "Theory of intermolecular pair correlations for molecular liquids. applications to the liquids carbon tetrachloride, carbon disulfide, carbon diselenide, and benzene," *J. Chem. Phys.*, vol. 61, no. 12, pp. 5228–5241, 1974.
- [119] B. M. Ladanyi and D. Chandler, "New type of cluster theory for molecular fluids: Interaction site cluster expansion," *J. Chem. Phys.*, vol. 62, no. 11, pp. 4308–4324, 1975.
- [120] J. D. Cox, "Phase relationships in the pyridine series. part ii. the miscibility of some pyridine homologues with deuterium oxide.," *J. Chem. Soc.*, p. 4606, 1952.
- [121] J. C. Crocker and D. G. Grier, "Methods of digital video microscopy for colloidal studies," *Journal of colloid and interface science*, vol. 179, no. 1, pp. 298–310, 1996.
- [122] J. N. Israelachvili, *Intermolecular and surface forces: revised third edition*. Academic press, 2011.
- [123] S. G. Stuij, M. Labbé-Laurent, T. E. Kodger, A. Maciołek, and P. Schall, "Critical casimir interactions of colloidal particles around the consolute point of binary solvents," *in preparation*, 2016.
- [124] R. L. Henderson, "A uniqueness theorem for fluid pair correlation functions," *Physics Letters A*, vol. 49, no. 3, pp. 197–198, 1974.
- [125] D. Chandler, "Cluster diagrammatic analysis of the rism equation," *Molecular Physics*, vol. 31, no. 4, pp. 1213–1223, 1976.
- [126] J. Talbot and D. J. Tildesley, "The planar dumbbell fluid," *J. Chem. Phys.*, vol. 83, pp. 6419–6424, 1985.
- [127] J.-P. Hansen and I. R. McDonald, *Theory of Simple Liquids*. Academic Press, San Diego, 2013.
- [128] D. Frenkel and B. Smit, *Understanding molecular simulation: from algorithms to applications*, vol. 1. Academic press, 2001.

-
- [129] G. A. Vliegenthart and H. N. W. Lekkerkerker, "Predicting the gas-liquid critical point from the second virial coefficient," *J. Chem. Phys.*, vol. 112, pp. 5364–5369, 2000.
- [130] H. C. Klein and U. S. Schwarz, "Studying protein assembly with reversible brownian dynamics of patchy particles," *The Journal of chemical physics*, vol. 140, no. 18, p. 184112, 2014.
- [131] Y. Y. Kuttner, N. Kozer, E. Segal, G. Schreiber, and G. Haran, "Separating the contribution of translational and rotational diffusion to protein association," *Journal of the American Chemical Society*, vol. 127, no. 43, pp. 15138–15144, 2005.
- [132] C. Li, Y. Wang, and G. J. Pielak, "Translational and rotational diffusion of a small globular protein under crowded conditions," *The Journal of Physical Chemistry B*, vol. 113, no. 40, pp. 13390–13392, 2009.
- [133] Y. Wang, C. Li, and G. J. Pielak, "Effects of proteins on protein diffusion," *Journal of the American Chemical Society*, vol. 132, no. 27, pp. 9392–9397, 2010.
- [134] D. Rapaport, "Role of reversibility in viral capsid growth: a paradigm for self-assembly," *Physical review letters*, vol. 101, no. 18, p. 186101, 2008.
- [135] A. C. Newton, J. Groenewold, W. K. Kegel, and P. G. Bolhuis, "Rotational diffusion affects the dynamical self-assembly pathways of patchy particles," *Proceedings of the National Academy of Sciences*, vol. 112, no. 50, pp. 15308–15313, 2015.
- [136] A. J. Williamson, A. W. Wilber, J. P. Doye, and A. A. Louis, "Templated self-assembly of patchy particles," *Soft Matter*, vol. 7, no. 7, pp. 3423–3431, 2011.
- [137] M. Nayhouse, V. R. Heng, A. M. Amlani, and G. Orkoulas, "Simulation of phase boundaries using constrained cell models," *Journal of Physics: Condensed Matter*, vol. 24, no. 37, p. 375105, 2012.
- [138] H. Liu, S. K. Kumar, and F. Sciortino, "Vapor-liquid coexistence of patchy models: relevance to protein phase behavior," *The Journal of chemical physics*, vol. 127, no. 8, p. 084902, 2007.
- [139] O. G. Berg and P. H. von Hippel, "Diffusion-controlled macromolecular interactions," *Annual review of biophysics and biophysical chemistry*, vol. 14, no. 1, pp. 131–158, 1985.
- [140] S. E. Halford and J. F. Marko, "How do site-specific dna-binding proteins find their targets?," *Nucleic acids research*, vol. 32, no. 10, pp. 3040–3052, 2004.

-
- [141] R. R. Gabdouliline and R. C. Wade, “On the protein-protein diffusional encounter complex,” *Journal of Molecular Recognition*, vol. 12, no. 4, pp. 226–234, 1999.
- [142] G. Schreiber, G. Haran, and H.-X. Zhou, “Fundamental aspects of protein-protein association kinetics,” *Chemical reviews*, vol. 109, no. 3, pp. 839–860, 2009.
- [143] G. Schreiber, “Kinetic studies of protein–protein interactions,” *Current opinion in structural biology*, vol. 12, no. 1, pp. 41–47, 2002.
- [144] L. Zhu, D. Frenkel, and P. G. Bolhuis, “Role of fluctuations in ligand binding cooperativity of membrane receptors,” *Physical review letters*, vol. 106, no. 16, p. 168103, 2011.
- [145] L. Colón-Meléndez, D. J. Beltran-Villegas, G. van Anders, J. Liu, M. Spellings, S. Sacanna, D. J. Pine, S. C. Glotzer, R. G. Larson, and M. J. Solomon, “Binding kinetics of lock and key colloids,” *The Journal of chemical physics*, vol. 142, no. 17, p. 174909, 2015.
- [146] A. C. Newton, A. Nguyen, S. J. Veen, D. Kraft, P. Schall, and P. G. Bolhuis, “Modelling critical casimir force induced self-assembly experiments on patchy colloidal dumbbells,” *submitted*, 2016.
- [147] C. Gögelein, G. Nägele, R. Tuinier, T. Gibaud, A. Stradner, and P. Schurtenberger, “A simple patchy colloid model for the phase behavior of lysozyme dispersions,” *The Journal of chemical physics*, vol. 129, no. 8, p. 085102, 2008.
- [148] C. Dellago, P. Bolhuis, and P. L. Geissler, “Transition path sampling,” *Advances in chemical physics*, vol. 123, no. 1, 2002.
- [149] P. G. Bolhuis and W. Lechner, “On the relation between projections of the reweighted path ensemble,” *Journal of Statistical Physics*, vol. 145, no. 4, pp. 841–859, 2011.
- [150] D. Chandler and J. D. Weeks, “Equilibrium structure of simple liquids,” *Physical review letters*, vol. 25, no. 3, p. 149, 1970.
- [151] J. D. Weeks, D. Chandler, and H. C. Andersen, “Role of repulsive forces in determining the equilibrium structure of simple liquids,” *The Journal of chemical physics*, vol. 54, no. 12, pp. 5237–5247, 1971.
- [152] A. Vijaykumar, P. G. Bolhuis, and P. R. ten Wolde, “Combining molecular dynamics with mesoscopic Green’s function reaction dynamics simulations,” *The Journal of chemical physics*, vol. 143, no. 21, p. 214102, 2015.