Publication List

Sergei A. Egorov

1. A. V. Tulub, V. F. Brattsev, and **S. A. Egorov**, "Nonempirical atomic potential method in the study of surface states of ionic crystals", Russ. J. Struct. Chem., **30**, p. 874-878 (1989).

2. R. A. Evarestov, V. P. Smirnov, and **S. A. Egorov**, "Band corepresentations of magnetic space-groups", Phys. Status Solidi B, **151**, p. 275-282 (1989).

3. **S. A. Egorov** and N. H. March, "Deformation of atomic density in a homonuclear diatomic molecule due to dispersion interaction", *Phys. Lett. A*, **157**, p. 57-59 (1991).

4. **S. A. Egorov** and N. H. March, "Model and experimental direct correlation functions in dense charged fluids", *Phys. Chem. Liq.*, **24**, p. 199-204 (1992).

5. **S. A. Egorov**, N. H. March and R. Santamaria, "Effects of exchange on equilibrium bond lengths of heavy, almost spherical, tetrahedral molecules XH_4", *Int. J. Quant. Chem.*, **42**, p. 1641-1649 (1992).

6. **S. A. Egorov** and N. H. March, "Transport properties of electron or hole liquids in the normal state of high-T_c copper oxides", *Phys. Chem. Liq.*, **27**, p. 195-198 (1994).

7. N. H. March, R. Pucci, and **S. A. Egorov**, "Limit of Fermi-liquid regime and binding energy of charged boson in high-T_c cuprates", *Phys. Chem. Liq.*, **28**, p. 141-144 (1994).

8. **S. A. Egorov** and N. H. March, "Dependence of transition temperature T_c on interlayer interaction via charged boson binding energy", *Phys. Chem. Liq.*, **30**, p. 59-62 (1995).

9. **S. A. Egorov** and J. L. Skinner, "On the theory of multiphonon relaxation rates in solids", *J. Chem. Phys.*, **103**, p. 1533-1543 (1995).

10. **S. A. Egorov**, M. D. Stephens, A. Yethiraj, and J. L. Skinner, "Structure and dynamics of infinitely dilute solutions", *Mol. Phys.*, **88**, p. 477-487 (1996).

11. **S. A. Egorov** and J. L. Skinner, "A theory of vibrational energy relaxation in liquids", *J. Chem. Phys.*, **105**, p. 7047-7058 (1996).

12. **S. A. Egorov** and J. L. Skinner, "An Improved theory of multiphonon relaxation in solids", *J. Chem. Phys.*, **105**, p. 10153-10155 (1996).

13. **S. A. Egorov** and J. L. Skinner, "Vibrational energy relaxation of diatomic molecules in rare gas crystals", *J. Chem. Phys.*, **106**, p. 1034-1040 (1997).

14. **S. A. Egorov**, M. D. Stephens, and J. L. Skinner, "Absorption line shapes and solvation dynamics of CH_3I in supercritical Ar", *J. Chem. Phys.*, **107**, p. 10485-10491 (1997).

15. **S. A. Egorov** and B. J. Berne, "Vibrational energy relaxation in condensed matter: quantum versus classical bath for multiphonon processes", *J. Chem. Phys.*, **107**, p. 6050-6061 (1997).

16. **S. A. Egorov**, E. Gallicchio, and B. J. Berne, "The simulation of electronic absorption spectrum of a chromophore coupled to a condensed phase environment: maximum entropy versus singular value decomposition approaches", *J. Chem. Phys.*, **107**, p. 9312-9318 (1997).

17. **S. A. Egorov**, E. Rabani, and B. J. Berne, "Vibronic spectra in condensed matter: a comparison of exact quantum mechanical and various semiclassical treatments for harmonic baths", *J. Chem. Phys.*, **108**, p. 1407-1422 (1998).

18. K. F. Everitt, **S. A. Egorov**, and J. L. Skinner, "Vibrational energy relaxation in liquid oxygen", *Chem. Phys.*, **235**, p. 115-122 (1998).

19. **S. A. Egorov**, and J. L. Skinner, "Semiclassical approximations to quantum time correlation functions", *Chem. Phys. Lett.*, **293**, p. 469-476 (1998).

20. E. Rabani, **S. A. Egorov**, and B. J. Berne, "A comparison of exact quantum mechanical and various semiclassical treatments for the vibronic absorption spectrum: The case of fast vibrational relaxation", *J. Chem. Phys.*, **109**, p. 6376-6381 (1998).

21. E. Gallicchio, **S. A. Egorov**, and B. J. Berne, "On the application of numerical analytic continuation methods to the study of quantum mechanical vibrational relaxation processes", *J. Chem. Phys.*, **109**, p. 7745-7755 (1998).

22. **S. A. Egorov**, E. Rabani, and B. J. Berne, "Nonradiative relaxation processes in condensed phases: Quantum versus classical baths" *J. Chem. Phys.*, **110**, p. 5238-5248 (1999).

23. E. Rabani, **S. A. Egorov**, and B. J. Berne, "Classical approximation to nonradiative electronic relaxation in condensed phases", *J. Phys. Chem. A*, **103**, p. 9539-9544 (1999).

24. **S. A. Egorov**, E. Rabani, and B. J. Berne, "On the adequacy of mixed quantum-classical dynamics in condensed phase systems" (Feature Article), *J. Phys. Chem. B*, **103**, p. 10978-10991 (1999).

25. **S. A. Egorov**, K. F. Everitt, and J. L. Skinner, "Quantum dynamics and vibrational relaxation", *J. Phys. Chem. A*, **103**, p. 9494-9499 (1999).

26. **S. A. Egorov**, "Preferential solvation in supercritical fluids: An integral equation study", *J. Chem. Phys.*, **113**, p. 7502-7510 (2000).

27. **S. A. Egorov**, "Local density augmentation in attractive supercritical solutions. II. Application to electronic line shifts", *J. Chem. Phys.*, **113**, p. 1950-1957 (2000).

28. **S. A. Egorov**, "Local density augmentation in attractive supercritical solutions: inhomogeneous fluid approach", *J. Chem. Phys.*, **112**, p. 7138-7146 (2000).

29. **S. A. Egorov** and J. L. Skinner, "Vibrational energy relaxation of polyatomic solutes in simple liquids and supercritical fluids", *J. Chem. Phys.*, **112**, p. 275-281 (2000).

30. **S. A. Egorov** and J. L. Skinner, "Vibrational line shifts in supercritical fluids", *J. Phys. Chem. A*, **104**, p. 483-489 (2000).

31. **S. A. Egorov**, A. Yethiraj, and J. L. Skinner, "Local density en-

hancement in dilute supercritical solutions", *Chem. Phys. Lett*, **317**, p. 558-566 (2000).

32. **S. A. Egorov**, "Adsorption of supercritical fluids and fluid mixtures: Inhomogeneous integral equation study", *J. Phys. Chem. B*, **105**, p. 6583-6591 (2001).

33. **S. A. Egorov** and E. Rabani, "Solute-solute potential of mean force in supercritical solutions: A nonlocal integral equation study", *J. Chem. Phys.*, **115**, p. 617-620 (2001).

34. E. Rabani and **S. A. Egorov**, "Interactions between passivated nanoparticles in solution: Beyond the continuum model", *J. Chem. Phys.*, **115**, p. 3437-3440 (2001).

35. E. Rabani and **S. A. Egorov**, "Integral equation theory for the interactions between passivated nanocrystals in supercritical fluids: Solvophobic and solvophilic cases", *J. Phys. Chem. B*, **106**, p. 6771-6778 (2002).

36. **S. A. Egorov** and E. Rabani, "Chemical equilibrium in supercritical fluids: Solvent effects on the dimerization equilibrium constants", *J. Chem. Phys.*, **116**, p. 8447-8454 (2002).

37. **S. A. Egorov**, R. A. Denny, and D. R. Reichman "On the multiple time scales in solvation dynamics: A mode-coupling theory approach", *J. Chem. Phys.*, **116**, p. 5080-5089 (2002).

38. **S. A. Egorov**, "Local density augmentation in attractive supercritical solutions. III. How important is the solute-solvent interaction range?", *J. Chem. Phys.*, **116**, p. 2004-2010 (2002).

39. **S. A. Egorov**, "Local density enhancement in neat supercritical fluids: Dependence on the interaction potential", *Chem. Phys. Lett.*, **354**, p. 140-147 (2002).

40. E. Rabani and **S. A. Egorov**, "Solvophobic and solvophilic effects on potential of mean force between two nanoparticles in binary mixtures", *Nanoletters*, **2**, p. 69-72 (2002).

41. **S. A. Egorov**, "A mode-coupling theory of diffusion in supercritical fluids", *J. Chem. Phys.*, **119**, p. 4798-4810 (2003).

42. **S. A. Egorov**, "Nonpolar solvation dynamics in supercritical fluids", *J. Chem. Phys.*, **118**, p. 10643-10650 (2003).

43. A. I. Chervanyov and **S. A. Egorov**, "Interaction between irreversibly adsorbed polymer layers: Is the mean field picture really inadequate?" *Phys. Rev. E*, **69**, p. 041801 (2004).

44. **S. A. Egorov**, "Ion solvation dynamics in supercritical fluids", *Phys. Rev. Lett.*, **93**, p. 023004 (2004).

45. N. Patel and **S. A. Egorov**, "Interactions between colloidal particles in polymer solution: A density functional theory study", *J. Chem. Phys.*, **121**, p. 4987-4997 (2004).

46. A. I. Chervanyov and **S. A. Egorov**, "A simple theory of the interaction between polymer brushes immersed in a supercritical fluid", *J. Chem. Phys.*, **121**, p. 6555-6560 (2004).

47. **S. A. Egorov**, "Solvation dynamics in supercritical fluids: Equilibrium versus nonequilibrium solvent response functions", *J. Chem. Phys.*, **121**, p. 6948-6955 (2004).

48. V. Kapko and **S. A. Egorov**, "Polar solvation dynamics in supercritical fluids: A mode-coupling treatment", *J. Chem. Phys.*, **121**, p. 11145-11155 (2004).

49. **S. A. Egorov**, "Effect of repulsive and attractive interactions on depletion forces in colloidal suspensions: A density functional theory treatment", *Phys. Rev. E*, **70**, p. 031402 (2004).

50. V. Kapko and **S. A. Egorov**, "Ion solvation in polar supercritical fluids: an integral equation study", *Chem. Phys. Lett.*, **402**, p. 258-264 (2005).

51. **S. A. Egorov**, "Interactions between nanoparticles in supercritical fluids: from repulsion to attraction", *Phys. Rev. E*, **72**, p. 010401 (2005).

52. N. Patel and **S. A. Egorov**, "Dispersing nanotubes with surfactants: A microscopic statistical mechanical analysis", *J. Am. Chem. Soc.*, **127**, p. 14124-14125 (2005).

53. **S. A. Egorov**, C. P. Lawrence, and J. L. Skinner, "A mode-coupling theory of vibrational line-broadening in near-critical fluids", *J. Phys. Chem. B*, **109**, p. 6879-6883 (2005).

54. N. Patel and **S. A. Egorov**, "Interactions between nanocolloidal particles in polymer solutions: Effect of attractive interactions", *J. Chem. Phys.*, **123**, p. 144916 (2005).

55. A. Striolo and **S. A. Egorov**, "Interactions between Sterically Stabilized Spherical Colloidal Particles: Implicit and Explicit Solvent", *J. Chem. Phys.*, **126**, p. 014902 (2007).

56. N. Patel and **S. A. Egorov**, "Interactions between Sterically Stabilized Nanoparticles in supercritical fluids: A Simulation Study", *J. Chem. Phys.*, **126**, p. 054706 (2007).

57. **S. A. Egorov**, "Interactions between Colloidal Particles in Amphiphilic Mixtures: A Density Functional Theory Study", *J. Chem. Phys.*, **127**, p. 184903 (2007).

58. C. N. Tiftickjian and **S. A. Egorov**, "Absorption and emission lineshapes and solvation dynamics of NO in supercritical Ar", *J. Chem. Phys.*, **128**, p. 114501 (2008).

59. **S. A. Egorov**, "A mode-coupling theory treatment of the transport coefficients of the Lennard-Jones fluid", *J. Chem. Phys.*, **128**, p. 144508 (2008).

60. **S. A. Egorov**, "Water-like Dynamic Anomalies in a Liquid Described by a Core-Softened Potential", *J. Chem. Phys.*, **128**, p. 174503 (2008).

61. **S. A. Egorov** and P. Larrégaray, "Absorption and Emission Lineshapes and Ultrafast Solvation Dynamics of NO in Parahydrogen", *J. Chem. Phys.*, **128**, p. 244502 (2008).

62. **S. A. Egorov**, "Structural and dynamical properties of a core-softened fluid in a supercitical region", *J. Chem. Phys.*, **129**, p. 024514

(2008).

63. **S. A. Egorov**, "Interactions between polymer brushes in solvents of variable quality: A density functional theory study", *J. Chem. Phys.*, **129**, p. 064901 (2008).

64. A. Milchev, **S. A. Egorov**, and K. Binder "Absorption/expulsion of oligomers and linear macromolecules in a polymer brush", *J. Chem. Phys.*, **132**, p. 184905 (2010).

65. L. A. Shall and **S. A. Egorov**, "Structural and dynamical anomalies of a Gaussian core fluid: A mode coupling theory study", *J. Chem. Phys.*, **132**, p. 184504 (2010).

66. F. Lo Verso, **S. A. Egorov**, A. Milchev, and K. Binder, "Spherical polymer brushes under good solvent conditions: Molecular dynamics results compared to density functional theory", *J. Chem. Phys.*, **133**, p. 184901 (2010).

67. **S. A. Egorov**, A. Milchev, L. Klushin, and K. Binder, "Structural properties of concave cylindrical brushes interacting with free chains", *Soft Matter*, **7**, p. 5669-5676, (2011).

68. F. LoVerso, L. Yelash, **S. A. Egorov**, and K. Binder, "Interactions between brush-coated spherical nanoparticles: The good solvent case", *J. Chem. Phys.*, **135**, p. 214902 (2011).

69. M. E. McEwan, **S. A. Egorov**, J. Ilavsky, D. L. Green, and Y. Yang, "Mechanical reinforcement of polymer nanocomposites: theory and ultra-small angle X-ray scattering (USAXS) studies", *Soft Matter*, **7**, p. 2725-2733, (2011).

70. **S. A. Egorov**, "Sterically stabilized lock and key colloids: A self-consistent field theory", *J. Chem. Phys.*, **134**, p. 194901 (2011).

71. **S. A. Egorov**, "Anomalous nanoparticle diffusion in polymer solutions and melts: A mode-coupling theory study", *J. Chem. Phys.*, **134**, p. 084903 (2011).

72. **S. A. Egorov**, "Hydrophobic interactions with coarse-grained model for water", *J. Chem. Phys.*, **134**, p. 234509 (2011).

73. **S. A. Egorov**, "Microphase separation of mixed polymer brushes physisorbed on cylindrical surfaces", *Soft Matter*, **8**, p. 3971-3979 (2012).

74. M. Camargo and **S. A. Egorov** and C. N. Likos, "Cluster formation in star-linear polymer mixtures: equilibrium and dynamical properties", *Soft Matter*, **8**, p. 4177-4184 (2012).

75. F. LoVerso, L. Yelash, **S. A. Egorov**, and K. Binder, "Effect of the solvent quality on the structural rearrangement of spherical brushes: coarse-grained models", Soft Matter, **8**, p. 4185-4196, (2012).

76. **S. A. Egorov** and K. Binder, "Effect of solvent quality on the dispersibility of polymer-grafted spherical nanoparticles in polymer solutions", J. Chem. Phys., **137**, p. 094901, (2012).

77. **S. A. Egorov**, D. Romeis, and J.-U. Sommer, "Surface instabilities of minority chains in dense polymer brushes: A comparison of density functional theory and quasi-off-lattice self-consistent field theory", J. Chem. Phys., **137**,

p. 064907, (2012).

78. F. LoVerso, **S. A. Egorov**, and K. Binder, "Interactions between brush-coated spherical nanoparticles: Effect of solvent quality", Macromolecules, **45**, p. 8892-8902, (2012).

79. **S. A. Egorov**, "Insertion of nanoparticles into polymer brush under variable solvent conditions", J. Chem. Phys., **137**, p. 134905, (2012).

80. R. Wang, **S. A. Egorov**, A. Milchev, and K. Binder, "Stretching of free chains confined in concave brush-coated nanocylinders", Macromolecules, **45**, p. 2580-2587, (2012).

81. F. A. M. Leermakers and **S. A. Egorov**, "On the collapse transition of a polymer brush: the case of lateral mobility", Soft Matter, **9**, p. 3341-3348, (2013).

82. **S. A. Egorov**, J. Paturej, C. N. Likos, and A. Milchev, "Controlling the Interactions between Soft Colloids via Surface Adsorption", Macromolecules, **46**, p. 3648-3653 (2013).

83. X. Z. Cao, H. Merlitz, C. X. Wu, **S. A. Egorov**, and J.-U. Sommer, "Effective Pair Potentials between Nanoparticles Induced by Single Monomers and Polymer Chains", Soft Matter, **9**, p. 5916-5926 (2013).

84. J. Paturej, A. Milchev, **S. A. Egorov**, and K. Binder "Star Polymers Confined in a Nanoslit: A Simulation Test of Scaling and Self-Consistent Field Theories", Soft Matter, **9**, p. 10522-10531 (2013).

85. J. Paturej, A. Milchev, **S. A. Egorov**, and K. Binder "The Escape Transition of a Compressed Star Polymer: Self-Consistent Field Predictions Tested by Simulation", Macromolecules, **46**, p. 8009-8016 (2013).

86. N. Dutta, **S. A. Egorov**, and D. Green, "Quantification of nanoparticle interactions in pure solvents and a concentrated PDMS solution as a function of solvent quality", Langmuir, **29**, p. 9991-10000 (2013).

87. A. Milchev, **S. A. Egorov**, and K. Binder, "Critical Adsorption of a Single Macromolecule into Polymer Brushes", Soft Matter, **10**, p. 5974-5990 (2014).

88. S. K. Das, **S. A. Egorov**, B. Trefz, P. Virnau, and K. Binder, "Phase behavior of active swimmers in depletants: Molecular dynamics and integral equation theory", Phys. Rev. Lett., **112**, p. 198301, (2014).

89. J. Riest, L. Athanasopoulou, **S. A. Egorov**, C. N. Likos and P. Ziherl, "Microelasticity of Deformable Nanocolloidal Particles", Sci. Rep., **112**, p. 15854, (2015).

90. **S. A. Egorov**, H. P. Hsu, A. Milchev, and K. Binder, "Semiflexible Polymer Brushes and the Brush-Mushroom Crossover", Soft Matter, **11**, p. 2604-2616 (2015).

91. Z. Farrell, S. Merz, J. Seager, C. Dunn, **S. A. Egorov**, and D. L. Green, "Development of Experiment and Theory to Detect and Predict Ligand Phase Separation on Silver Nanoparticles", Angewandte Chemie, **54**, p. 6479-6482, (2015).

92. B. Trefz, S. K. Das, **S. A. Egorov**, P. Virnau, and K. Binder, "Activity mediated phase separation: Can we understand phase behavior

of the nonequilibrium problem from an equilibrium approach?", J. Chem. Phys., **144**, p. 144902, (2016).

93. **S. A. Egorov**, A. Milchev, P. Virnau, and K. Binder, "Semiflexible polymers under good solvent conditions interacting with repulsive walls", J. Chem. Phys., **144**, p. 174902, (2016).

94. **S. A. Egorov**, A. Milchev, and K. Binder, "Anomalous fluctuations of nematic order in solutions of semiflexible polymers", Phys. Rev. Lett., **116**, p. 187801, (2016).

95. **S. A. Egorov**, A. Milchev, P. Virnau, and K. Binder, "A New Insight into the Isotropic - Nematic phase transition in lyotropic solutions of semiflexible polymers: Density-Functional Theory tested by Molecular Dynamics", Soft Matter, **12**, p. 4944-4959, (2016).

96. P. Poier, **S. A. Egorov**, C. N. Likos, and R. Blaak, "Concentration-induced Planar-to-homeotropic Anchoring Transition of Stiff Ring Polymers on Hard Walls", Soft Matter, **12**, p. 7983-7994, (2016).

97. **S. A. Egorov**, A. Milchev, and K. Binder, "Semiflexible Polymers in the Bulk and Confined by Planar Walls", Polymers, **8**, p. 296, (2016).

98. **S. A. Egorov**, A. Milchev, and K. Binder, "Semiflexible Polymers Confined between Repulsive Walls: A Density Functional and Molecular Dynamics Simulation Study of Capillary Nematization", Macromol. Theory and Simulations, **25**, p. 1600036, (2017).

99. H. Popova, A. Milchev, and **S. A. Egorov**, "Modeling the Interfacial Tension Dependence on Composition and Stiffness of Nonionic Surfactants on Liquid-Liquid Interfaces", Coll. Surf. A, **509**, p. 168-178 (2017).

100. P. E. Theodorakis, **S. A. Egorov**, and A. Milchev, "Stiffness-guided motion of a droplet on a solid substrate", *J. Chem. Phys.*, **146**, p. 244705 (2017).

101. A. Milchev, **S. A. Egorov**, A. Nikoubashman, and K. Binder, "Conformations and orientational ordering of semiflexible polymers in pherical confinement", *J. Chem. Phys.*, **146**, p. 194907 (2017).

102. A. Milchev, **S. A. Egorov**, D. A. Vega, K. Binder, and A. Nikoubashman, "Densely Packed Semiflexible Macromolecules in a Rigid Spherical Capsule", *Macromolecules*, **51**, p. 20022016 (2018).

103. K. Binder, **S. A. Egorov**, and A. Milchev "Polymer Brushes on Flat and Curved Substrates: What Can be Learned from Molecular Dynamics Simulations", *in book*, **Polymer and Biopolymer Brushes for Materials Science and Biotechnology**, p. 141-159, Editors: O. Azzaroni and I. Szleifer, Wiley (2018).

104. A. Milchev, **S. A. Egorov**, A. Nikoubashman, and K. Binder, "Adsorption and structure formation of semiflexible polymers on spherical surfaces", *Polymer*, **145**, p. 463-472, (2018).

105. S. K. Das, **S. A. Egorov**, P. Virnau, D. Winter, and K. Binder, "Do the contact angle and line tension of surface-attached droplets depend on the radius of curvature?", *J. Phys. Cond. Matt.*, **30**, p. 255001 (2018).

106. M. Bottcher, S. Heinze, **S. A. Egorov**, J. Sinova and B. Dupe, "B-T phase diagram of Pd/Fe/Ir(111) computed with parallel tempering Monte Carlo", *New J. Phys.*, **20**, p. 103014 (2018).

107. S. N. Merz, Z. J. Farrell, J. Pearring, E. Hoover, M. Kester, **S. A. Egorov**, D. L. Green, and K. H. DuBay, "Computational and Experimental Investigation of Janus-like Monolayers on Ultrasmall Noble Metal Nanoparticles", *ACS Nano*, **12**, p. 11031-11040, (2018).

108. A. Milchev, **S. A. Egorov**, A. Nikoubashman, and K. Binder, "Nematic order in solutions of semiflexible polymers: Hairpins, elastic constants, and the nematic-smectic transition", *J. Chem. Phys.*, **149**, p. 174909, (2018).

109. K. E. Klop, R. P. A. Dullens, M. P. Lettinga, **S. A. Egorov**, and D. G. A. L. Aarts, "Capillary nematisation of colloidal rods in confinement", *Mol. Phys.*, **116**, p. 2864-2871, (2018).

110. R. J. Chen, R. Poling-Skutvik, M. P. Howard, A. Nikoubashman, **S. A. Egorov**, J. C. Conrad, and J. C. Palmer, "Influence of polymer flexibility on nanoparticle dynamics in semidilute solutions", *Soft Matter*, **15**, p. 1260-1268, (2019).

111. S. J. Wang, D. Venkateshvaran, M. R. Mahani, U. Chopra, E. R. McNellis, R. Di Pietro, S. Schott, A. Wittmann, G. Schweicher, M. Cubukcu, K. Kang, R. Carey, T. J. Wagner, J. N. M. Siebrecht, D. P. G. H. Wong, I. E. Jacobs, R. O. Aboljadayel, A. Ionescus, **S. A. Egorov**, S. Mueller, O. Zadvorna, P. Skalski, C. Jellett, M. Little, A. Marks, I. McCulloch, J. Wunderlich, J. Sinova, H. Sirringhaus, "Long spin diffusion lengths in doped conjugated polymers due to enhanced exchange coupling", *Nature Electronics*, **2**, p. 98-107, (2019).

112. J. Midya, Y. Cang, **S. A. Egorov**, K. Matyjaszewski, M. R. Bockstaller, A. Nikoubashman, and G. Fytas, "Disentangling the Role of Chain Conformation on the Mechanics of Polymer Tethered Particle Materials", *Nano Letters*, **19**, p. 2715-2722, (2019).

113. S. N. Merz, E. Hoover, **S. A. Egorov**, K. H. DuBay, and D. L. Green, "Predicting the effect of chain-length mismatch on phase separation in noble metal nanoparticle monolayers with chemically mismatched ligands", *Soft Matter*, **15**, p. 4498-4507 (2019).

114. J. Midya, **S. A. Egorov**, K. Binder, and A. Nikoubashman, "Phase behavior of flexible and semiflexible polymers in solvents of varying quality", *J. Chem. Phys.*, **151**, p. 034902 (2019).

115. U. Chopra, **S. A. Egorov**, J. Sinova, and E. R. McNellis, "Chemical and structural trends in the spin-admixture parameter of organic semiconductor molecules", *J. Phys. Chem. C*, **123**, p. 19112-19118 (2019).

116. U. Chopra, S. Shambhawi, **S. A. Egorov**, J. Sinova, and E. R. McNellis, "Accurate and general formalism for spin-mixing parameter calculations", *Phys. Rev. B*, **100**, p. 134410 (2019).