Estimating the density of deep eutectic solvents applying supervised machine learning techniques (/paperRedirect/1506706873396346880)

Scientific Reports (/paper/journal/55?r_detail=1506706873396346880) (IF 4.379) **Pub Date : 2022-03-23** , DOI: 10.1038/s41598-022-08842-5 (/paperRedirect/1506706873396346880)

Mohammadjavad Abdollahzadeh, Marzieh Khosravi, Behnam Hajipour Khire Masjidi, Amin Samimi Behbahan, Ali Bagherzadeh, Amir Shahkar, Farzad Tat Shahdost

Deep eutectic solvents (DES) are recently synthesized to cover limitations of conventional solvents. These green solvents have wide ranges of potential usages in real-life applications. Precise measuring or accurate estimating thermophysical properties of DESs is a prerequisite for their successful applications. Density is likely the most crucial affecting characteristic on the solvation ability of DESs. This study utilizes seven machine learning techniques to estimate the density of 149 deep eutectic solvents. The density is anticipated as a function of temperature, critical pressure and temperature, and acentric factor. The LSSVR (least-squares support vector regression) presents the highest accuracy among 1530 constructed intelligent estimators. The LSSVR predicts 1239 densities with the mean absolute percentage error (MAPE) of 0.26% and R^2 = 0.99798. Comparing the LSSVR and four empirical correlations revealed that the earlier possesses the highest accuracy level. The prediction accuracy of the LSSVR (i.e., MAPE = 0. 26%) is 74.5% better than the best-obtained results by the empirical correlations (i.e., MAPE = 1.02%).

中文翻译：

中文翻译由计算机程序完成，如与英文原文有差异，以后者为准

应用监督机器学习技术估计深共熔溶剂的密度

最近合成了深共熔溶剂 (DES)，以弥补传统溶剂的局限性。这些绿色溶剂在实际应用中具有广泛的潜在用途。精确测量或准确估计 DES 的热物理性质是其成功应用的先决条件。密度可能是影响 DES 溶剂化能力的最关键特征。本研究利用七种机器学习技术来估计 149 种深共熔溶剂的密度。预计密度是温度、临界压力和温度以及无心因素的函数。LSSVR (最小二乘支持向量回归) 在 1530 个构建的智能估计器中表现出最高的准确度。LSSVR 预测 1239 个密度，平均绝对百分比误差 (MAPE) 为 0.26%，R^2 = 0.99798。比较 LSSVR 和四个经验相关性表明，较早的具有最高的准确度水平。LSSVR 的预测精度 (即 MAPE = 0. 26%) 比经验相关性获得的最佳结果 (即 MAPE = 1.02%) 好 74.5%。

更新日期：2022-03-23

点击分享 查看原文 (/paperRedirect/1506706873396346880) 点击收藏
阅读更多本刊最新论文 (/paper/journal/55?r_detail=1506706873396346880) 本刊介绍/投稿指南 (/8paper/1201710381848662016?r_detail=1506706873396346880)

相关文章

Chemical vapor deposition of 2D materials: A review of modeling, simulation, and machine learning studies (/paper/1487999775438397440?recommendPaper=1506706873396346880) (/paper/1487999775438397440?recommendPaper=1506706873396346880) (/paper/1487999775438397440?recommendPaper=1506706873396346880) *iScience* (/paper/journal/1314?recommendPaper=150... Sayan Bhowmik, Ananth Govind Rajan (/paper/1487999775438397440?recommendPaper=1506706873396346880)

Engineering chemistry to meet COP26 targets (/paper/1466851803428069376?recommendPaper=1506706873396346880) (/paper/1466851803428069376?recommendPaper=1506706873396346880)

全部期刊列表>>
(/paper/list)

(/paper/14668518034280693 76?recommendPaper=1506706873396346880) *Nature Reviews Chemistry* (/paper/journal/134?recom...
Anthony J. Ryan, Rachael H. Rothman
(/paper/14668518034280693 76?recommendPaper=1506706873396346880)

Augmenting zero-Kelvin quantum mechanics with machine learning for the prediction of chemical reactions at high temperatures (/paper/1466138986503110656?recommendPaper=1506706873396346880) (/paper/1466138986503110656?recommendPaper=1506706873396346880)
(/paper/1466138986503110656?recommendPaper=1506706873396346880) *Nature Communications* (/paper/journal/49?recomme...
Jose Antonio Garrido Torres, Vahe Gharakhanyan, Nongnuch Artrith, Tobias Hoffmann Eegholm, Alexander Urban
(/paper/1466138986503110656?recommendPaper=1506706873396346880)

Tunable and functional deep eutectic solvents for lignocellulose valorization (/paper/1437850851443798016?recommendPaper=1506706873396346880) (/paper/1437850851443798016?recommendPaper=1506706873396346880)
(/paper/1437850851443798016?recommendPaper=1506706873396346880) *Nature Communications* (/paper/journal/49?recomme...
Yongzhuang Liu, Noemi Deak, Zhiwen Wang, Haipeng Yu, Lisanne Hameleers, Edita Jurak, Peter J. Deuss, Katalin Barta
(/paper/1437850851443798016?recommendPaper=1506706873396346880)

Density, viscosity, surface tension, spectroscopic properties and computational chemistry of the 1, 4-butanediol + 1, 3-propanediamine-based deep eutectic solvent (/paper/1504190505068421120?recommendPaper=1506706873396346880)
(/paper/1504190505068421120?recommendPaper=1506706873396346880)
(/paper/1504190505068421120?recommendPaper=1506706873396346880) *Journal of the Iranian Chemical Society* (/paper/journal...
Kun Liu, Bin Li, Rumeng Zhang, Ying Zhang, Jianbin Zhang
(/paper/1504190505068421120?recommendPaper=1506706873396346880)

Deep Eutectic Solvents and Multicomponent Reactions: Two Convergent Items to Green Chemistry Strategies (/paper/1427740469920251904?recommendPaper=1506706873396346880) (/paper/1427740469920251904?recommendPaper=1506706873396346880)
(/paper/1427740469920251904?recommendPaper=1506706873396346880) *ChemistryOpen* (/paper/journal/1743?recommendPap...
Francisco G. Calvo-Flores, Cristina Mingorance-Sánchez
(/paper/1427740469920251904?recommendPaper=1506706873396346880)

Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems (/paper/1412880575481712640?recommendPaper=1506706873396346880) (/paper/1412880575481712640?recommendPaper=1506706873396346880)
(/paper/1412880575481712640?recommendPaper=1506706873396346880) *Chemical Reviews* (/paper/journal/44?recommendPap...
John A. Keith, Valentin Vassilev-Galindo, Bingqing Cheng, Stefan Chmiela, Michael Gastegger, Klaus-Robert Müller, Alexandre Tkatc...
(/paper/1412880575481712640?recommendPaper=1506706873396346880)

Deepometry, a framework for applying supervised and weakly supervised deep learning to imaging cytometry (/paper/1406028814827859968?recommendPaper=1506706873396346880) (/paper/1406028814827859968?recommendPaper=1506706873396346880)
(/paper/1406028814827859968?recommendPaper=1506706873396346880) *Nature Protocols* (/paper/journal/387?recommendPap...
Minh Doan, Claire Barnes, Claire McQuin, Juan C. Caicedo, Allen Goodman, Anne E. Carpenter, Paul Rees
(/paper/1406028814827859968?recommendPaper=1506706873396346880)

Inorganic Synthesis Based on Reactions of Ionic Liquids and Deep Eutectic Solvents (/paper/1397303322543112192?recommendPaper=1506706873396346880) (/paper/1397303322543112192?recommendPaper=1506706873396346880)
(/paper/1397303322543112192?recommendPaper=1506706873396346880) *Angewandte Chemie International Edition* (/paper/jour...
Tao Zhang, Thomas Doert, Hui Wang, Suojiang Zhang, Michael Ruck
(/paper/1397303322543112192?recommendPaper=1506706873396346880)

Group contribution and atomic contribution models for the prediction of various physical properties of deep eutectic solvents (/paper/1374427242654285824?recommendPaper=1506706873396346880) (/paper/1374427242654285824?recommendPaper=1506706873396346880)
(/paper/1374427242654285824?recommendPaper=1506706873396346880) *Scientific Reports* (/paper/journal/55?recommendPape...
Reza Haghbakhsh, Sona Raeissi, Ana Rita C. Duarte
(/paper/1374427242654285824?recommendPaper=1506706873396346880)

Corrigendum: Deep Eutectic Supramolecular Polymers: Bulk Supramolecular Materials (/paper/1366507864686424064?recommendPaper=1506706873396346880) (/paper/1366507864686424064?recommendPaper=1506706873396346880)
(/paper/1366507864686424064?recommendPaper=1506706873396346880) *Angewandte Chemie International Edition* (/paper/jour...

Shuanggen Wu, Changyong Cai, Fenfang Li, Zhijian Tan, Shengyi Dong
(/paper/1366507864686424064?recommendPaper=1506706873396346880)

Applying Machine Learning to Balance Performance and Stability of High Energy Density Materials (/paper/1365438314565955584?recommendPaper=1506706873396346880) (/paper/1365438314565955584?recommendPaper=1506706873396346880)
(/paper/1365438314565955584?recommendPaper=1506706873396346880) *iScience* (/paper/journal/1314?recommendPaper=150...
Xiaona Huang, Chongyang Li, Kaiyuan Tan, Yushi Wen, Feng Guo, Ming Li, Yongli Huang, Chang Q. Sun, Michael Gozin, Lei Zhang
(/paper/1365438314565955584?recommendPaper=1506706873396346880)

Advances in engineering near-infrared luminescent materials (/paper/1358612865555931136?recommendPaper=1506706873396346880) (/paper/1358612865555931136?recommendPaper=1506706873396346880)
(/paper/1358612865555931136?recommendPaper=1506706873396346880) *iScience* (/paper/journal/1314?recommendPaper=150...
Christopher T. Jackson, Sanghwa Jeong, Gabriel F. Dorlhiac, Markita P. Landry
(/paper/1358612865555931136?recommendPaper=1506706873396346880)

Convergence of multiple synthetic paradigms in a universally programmable chemical synthesis machine (/paper/1341520460778225664?recommendPaper=1506706873396346880) (/paper/1341520460778225664?recommendPaper=1506706873396346880)
(/paper/1341520460778225664?recommendPaper=1506706873396346880) *Nature Chemistry* (/paper/journal/3?recommendPaper...
Davide Angelone, Alexander J. S. Hammer, Simon Rohrbach, Stefanie Krambeck, Jarosław M. Granda, Jakob Wolf, Sergey Zalesskiy, ...
(/paper/1341520460778225664?recommendPaper=1506706873396346880)

Microextraction Techniques with Deep Eutectic Solvents (/paper/1340520943220080640?recommendPaper=1506706873396346880) (/paper/1340520943220080640?recommendPaper=1506706873396346880)
(/paper/1340520943220080640?recommendPaper=1506706873396346880) *Molecules* (/paper/journal/1351?recommendPaper=15...
Orfeas-Evangelos Plastiras, Eirini Andreasidou, Victoria Samanidou
(/paper/1340520943220080640?recommendPaper=1506706873396346880)

Meta-analysis of viscosity of aqueous deep eutectic solvents and their components (/paper/1336021973132763136?recommendPaper=1506706873396346880) (/paper/1336021973132763136?recommendPaper=1506706873396346880)
(/paper/1336021973132763136?recommendPaper=1506706873396346880) *Scientific Reports* (/paper/journal/55?recommendPape...
Gudrun Gygli, Xinmeng Xu, Jürgen Pleiss
(/paper/1336021973132763136?recommendPaper=1506706873396346880)

Deep eutectic solvents for solid pesticide dosage forms (/paper/1332171583051177984?recommendPaper=1506706873396346880) (/paper/1332171583051177984?recommendPaper=1506706873396346880)
(/paper/1332171583051177984?recommendPaper=1506706873396346880) *Scientific Reports* (/paper/journal/55?recommendPape...
Justin Phillips, Walter W. Focke, Elizabeth L. du Toit, James Wesley-Smith
(/paper/1332171583051177984?recommendPaper=1506706873396346880)

Chemist versus Machine: Traditional Knowledge versus Machine Learning Techniques (/paper/1326768528466026496?recommendPaper=1506706873396346880) (/paper/1326768528466026496?recommendPaper=1506706873396346880)
(/paper/1326768528466026496?recommendPaper=1506706873396346880) *Trends in Chemistry* (/paper/journal/1481?recommend...
Janine George, Geoffroy Hautier
(/paper/1326768528466026496?recommendPaper=1506706873396346880)

Quantum chemical accuracy from density functional approximations via machine learning (/paper/1317595469378195456?recommendPaper=1506706873396346880) (/paper/1317595469378195456?recommendPaper=1506706873396346880)
(/paper/1317595469378195456?recommendPaper=1506706873396346880) *Nature Communications* (/paper/journal/49?recomme...
Mihail Bogojeski, Leslie Vogt-Maranto, Mark E. Tuckerman, Klaus-Robert Müller, Kieron Burke
(/paper/1317595469378195456?recommendPaper=1506706873396346880)

Deep learning chemistry ab initio (/paper/1311366469744037888?recommendPaper=1506706873396346880)
(/paper/1311366469744037888?recommendPaper=1506706873396346880)
(/paper/1311366469744037888?recommendPaper=1506706873396346880) *Nature Reviews Chemistry* (/paper/journal/134?recom...
Gabriella Graziano
(/paper/1311366469744037888?recommendPaper=1506706873396346880)

我有话说~~

评论

客服邮箱：service@x-mol.com (mailTo:service@x-mol.com)
官方微信：X-molTeam2
邮编：100098
地址：北京市海淀区知春路56号中航科技大厦

扫一扫下载APP

X-MOL公众号