

## Front Cover

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## Back Cover

See Chen Yang, Ting Qiu *et al.*,  
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#### COSMO-based models

Zhigang Lei, Zhiwen Qi, Chengna Dai, Jose Palomar..... 309

### Research highlight

#### COSMO-based models for predicting the gas solubility in polymers

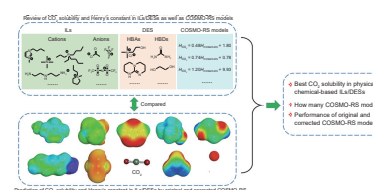
Ruisong Zhu, Zhigang Lei\*..... 311

### Research papers

#### Ionic liquids/deep eutectic solvents for CO<sub>2</sub> capture: Reviewing and evaluating

Yanrong Liu, Zhengxing Dai, Zhibo Zhang, Shaojuan Zeng, Fangfang Li, Xiangping Zhang, Yi Nie, Lei Zhang, Suojiang Zhang\*, Xiaoyan Ji\*..... 314

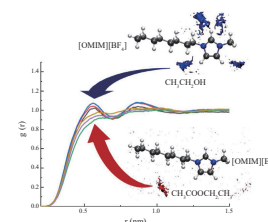
The CO<sub>2</sub> solubility (including Henry's constant) in ILs/DESs and the COSMO-RS models describing these properties were collected, and compared with the original and corrected COSMO-RS prediction results. Then the best CO<sub>2</sub> solubility and the performance of COSMO-RS models were achieved.



#### Molecular interaction mechanism in the separation of a binary azeotropic system by extractive distillation with ionic liquid

Hong Li, Guanlun Sun, Dongyang Li, Li Xi\*, Peng Zhou, Xingang Li, Ji Zhang, Xin Gao\*..... 329

The preferred ionic liquid screened by COSMO-RS is proved as a promising extracting agent in the extractive distillation of a binary azeotropic system. With quantum mechanics and molecular dynamics simulation, the separation mechanism of extractive distillation was explored from molecular level.

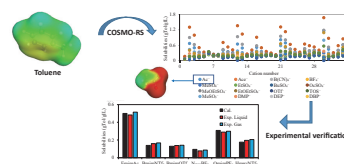


# Green Energy & Environment

## Study of the toluene absorption capacity and mechanism of ionic liquids using COSMO-RS prediction and experimental verification

Chenglong Zhang, Jin Wu, Ruixue Wang\*, En Ma, Liang Wu, Jianfeng Bai, Jingwei Wang..... 339

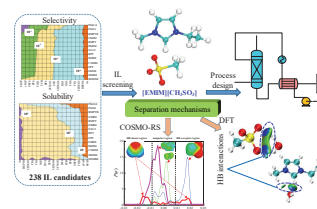
In the present study, the solubility of toluene in 816 ILs was predicted by COSMO-RS, furthermore, the experimental verification and mechanism were discussed, which could provide a fundamental basis and practical data for the control and treatment of VOCs.



## Chlorine drying with hygroscopic ionic liquids

Gangqiang Yu, Chengna Dai, Bin Wu, Ning Liu, Biaohua Chen, Ruinian Xu\*..... 350

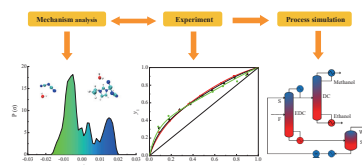
A new Cl<sub>2</sub> drying technology with IL is proposed. The hygroscopic IL [EMIM][CH<sub>3</sub>SO<sub>3</sub>] is selected from various IL candidates as a very promising alternative absorbent to conventional concentrated sulfuric acid for highly efficient Cl<sub>2</sub> drying.



## [EMIM][DCA] as an entrainer for the extractive distillation of methanol-ethanol-water system

Shengli Liu, Zhenhang Wang, Ruisong Zhu, Zhigang Lei, Jiqin Zhu\*..... 363

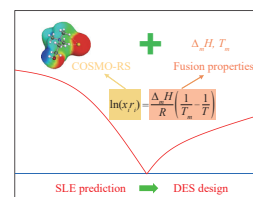
The COSMO-RS model was applied to screen out the appropriate entrainer and explain the separation mechanism. With the phase behaviors and energy consumption of separation process predicted according to UNIFAC model, this work ranges from molecular level to systematic scale.



## Evaluation of COSMO-RS for solid-liquid equilibria prediction of binary eutectic solvent systems

Zhen Song\*, Jingwen Wang, Kai Sundmacher ..... 371

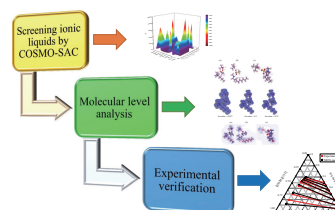
The solid-liquid equilibria prediction by COSMO-RS provides a promising way to the theoretical design of (deep) eutectic solvent. With the identified calculation option and applicability range of COSMO-RS, new eutectic solvents could be readily explored.



## Separation of n-heptane and tert-butanol by ionic liquids based on COSMO-SAC model

Zhengrun Chen, Hongru Zhang, Huiyuan Li, Ying Xu, Yuanyuan Shen, Zhaoyou Zhu, Jun Gao, Yixin Ma, Yinglong Wang\*..... 380

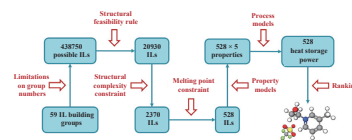
Three imidazolium ionic liquids were determined from 100 ionic liquids by COSMO-SAC to separate n-heptane/tert-butanol system and further verified experimentally. 1-hexyl-3-methylimidazolium tetrafluoromethanesulfonate ([HMIM][OTF]) shows the best performance and its mechanism is explained by interaction energy and charge density.



## Model-based optimal design of phase change ionic liquids for efficient thermal energy storage

Huaiwei Shi, Xiang Zhang, Kai Sundmacher, Teng Zhou\* ..... 392

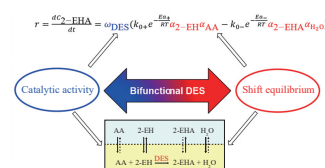
Using the computer-aided molecular design (CAMD) method, the best phase-change ionic liquid [MPyEtOH][TfO] is identified for efficient thermal energy storage. This material shows a higher heat storage performance than the traditional phase-change material paraffin wax.



## Reactive extraction for intensifying 2-ethylhexyl acrylate synthesis using deep eutectic solvent [Im:2PTSA]

Ruizhuan Wang, Hao Qin, Jingwen Wang, Hongye Cheng\*, Lifang Chen, Zhiwen Qi\* ..... 405

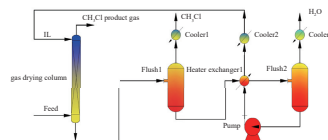
Reactive extraction is proposed for 2-ethylhexyl acrylate synthesis intensified by bifunctional deep eutectic solvent (DES), the role as catalyst and extractant is verified by thermodynamic analysis and kinetic modeling.



## Methyl chloride dehydration with ionic liquid based on COSMO-RS model

Zhenhang Wang, Shengli Liu, Yifan Jiang, Zhigang Lei, Jie Zhang\*, Ruisong Zhu, Jiwen Ren ..... 413

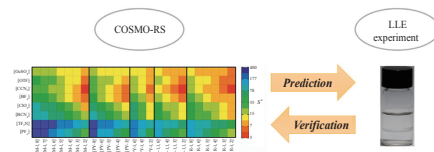
The ionic liquid [EMIM][BF<sub>4</sub>] with strong hydrophilic ability are used to dry methyl chloride gas. The two flashing operations are used to separate methyl chloride and water in the recovery process of the ionic liquid [EMIM][BF<sub>4</sub>].



## COSMO-RS prediction and experimental verification of 1,5-pentanediamine extraction from aqueous solution by ionic liquids

Chenhao Jiang, Hongye Cheng\*, Zexian Qin, Ruizhuan Wang, Lifang Chen, Chen Yang, Zhiwen Qi\*, Xiucui Liu ..... 422

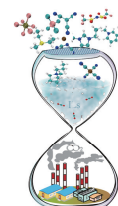
COSMO-RS model was used to predict the performance of 200 ionic liquids in the extraction of 1,5-pentanediamine from aqueous solution. Experimental liquid-liquid equilibrium experiments demonstrated the effects of cation and anion on extraction performance and verified the reliability of COSMO-RS model in ionic liquid screening for 1,5-pentanediamine extraction.



## Machine learning-based ionic liquids design and process simulation for CO<sub>2</sub> separation from flue gas

Kai Wang, Huijin Xu, Chen Yang\*, Ting Qiu\* ..... 432

The optimal ionic liquids are designed, selected and evaluated by the COSMO-RS model, support vector machine model and industrial process simulation, respectively, to apply for CO<sub>2</sub> separation from the flue gas.



## Extractive distillation of the benzene and acetonitrile mixture using an ionic liquid as the entrainer

Yichun Dong, Qingchun Yang, Zhiwei Li, Zhigang Lei\* ..... 444

The suitable ionic liquid of the separation of the benzene and acetonitrile mixture by extractive distillation was selected by the COSMO-RS model, and 1-ethyl-3-methylimidazolium tetrafluoroborate ([EMIM][BF<sub>4</sub>]) was considered as the suitable entrainer mainly due to its high selectivity, low viscosity, and low price.

