

# 学术文献阅读

2020年9月5日

# 目录

□ 文献获取

□ 文献管理

□ 文献阅读

# 文献获取

- 搜索关键词
- 人名/课题组
- 跟踪订阅
- 他人推荐
- 已有文献拓展

# 文献获取-关键词



➤ Google scholar



➤ Scopus

➤ Web of science

# 文献获取-人名搜索

- Google scholar citation
- Homepage
- Researchgate



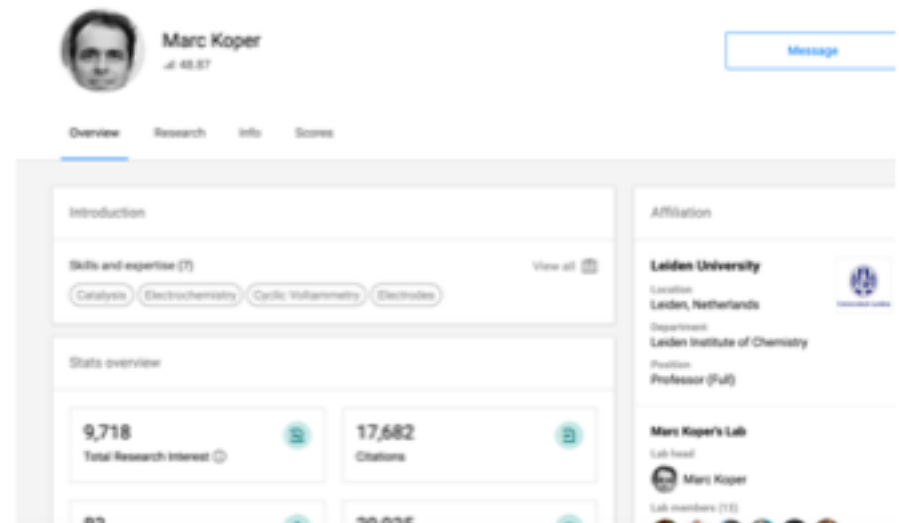
ResearchGate profile of Marc Koper. The profile shows a blue graduation cap icon, the name "Marc Koper", and the affiliation "Unknown affiliation". Below the profile information is a table of publications.

Title	Cited by	Year
Catalysis and reaction pathways for the electrochemical reduction of carbon dioxide B. Kuhlmann, J. Shen, M.P. Schuster, F. Gutzler, M.P. Schuster The Journal of Physical Chemistry Letters 1 (2010) 4073-4082	497	2010
Thermodynamic theory of multi-electron transfer reactions: Implications for electrocatalysis M.P. Schuster Journal of Electroanalytical Chemistry 690 (2012) 204-205	447	2011
Nitrogen cycle electrocatalysis M. Koper, M. Koper, M.P. Schuster, M.P. Schuster Chemical Reviews 109 (5) 2009-2044	405	2009
A new mechanism for the selectivity to C 1 and C 2 species in the electrochemical reduction of carbon dioxide on copper electrodes M.P. Schuster, T. Koper, G. van der Wal, M. Koper Chemical Science 2 (10) 1952-1960	366	2011
Role of crystalline defects in electrocatalysis: Mechanism and kinetics of CO adsorption on stepped platinum electrodes M.P. Schuster, M.P. Schuster, M.P. Schuster, M.P. Schuster The Journal of Physical Chemistry B 116 (20) 12008-12017	307	2012
Electrocatalytic reduction of nitrate at low concentration on coinage and transition-metal electrodes in acid solutions M. Koper, M.P. Schuster, M.P. Schuster Journal of Electroanalytical Chemistry 594, 10-21	219	2010



Google Scholar profile of Marc Koper. The profile shows a photo of Marc Koper, his name, and his title "Professor of Catalysis and surface chemistry". Below the profile information is a table of publications.

Publication	Cited by	Year
Bonds, C. J., Calle-Vallejo, F., Costa-Figueroa, M., & Koper, M. T. M. (2010). Structural principles to steer the selectivity of the electrocatalytic reduction of aliphatic ketones on platinum. <i>Nature Catalysis</i> 2(3), 243-250. article in journal - referenced		
Bongers, M. J., Calle-Vallejo, F., Koper, M. T. M., Hermers, E., & Feliu, J. M. (2010). Electrocatalytic enhancement of formic acid oxidation reaction by adsorbate on well-defined platinum surfaces. <i>Electrochimica Acta</i> 55, 835-845. article in journal - referenced		



ResearchGate profile of Marc Koper. The profile shows a photo of Marc Koper, his name, and his title "Professor of Catalysis and surface chemistry". Below the profile information is a table of publications.

Publication	Cited by	Year
Bonds, C. J., Calle-Vallejo, F., Costa-Figueroa, M., & Koper, M. T. M. (2010). Structural principles to steer the selectivity of the electrocatalytic reduction of aliphatic ketones on platinum. <i>Nature Catalysis</i> 2(3), 243-250. article in journal - referenced		
Bongers, M. J., Calle-Vallejo, F., Koper, M. T. M., Hermers, E., & Feliu, J. M. (2010). Electrocatalytic enhancement of formic acid oxidation reaction by adsorbate on well-defined platinum surfaces. <i>Electrochimica Acta</i> 55, 835-845. article in journal - referenced		

# 文献获取-订阅



Marc Koper

Unknown affiliation  
No verified email

FOLLOW



Scopus

检索 来源出版物 列表 SciVal >



创建帐户

## 作者详情

Koper, Marc T.M.

查看可能的匹配作者

作者 ID: 7006205398

归属机构:

Leiden Institute of Chemistry, Leiden, Netherlands 查看更多

其他姓名格式:

Koper, Marc Koper, M. Koper, M. T.M.

学科类别:

Chemistry Chemical Engineering Physics and Astronomy Materials Science Energy Biochemistry, Genetics and Molecular Biology Engineering Environmental Science Mathematics Multidisciplinary

按作者的文献

386

分析作者的产出

总引文献

按 13198 文献分组的 24503

查看引文概览

$h$ -index:

84

查看  $h$ -graph

## 个人资料操作

编辑作者个人资料

连接到 ORCID

Alerts  
设置引文通知  
设置文献通知

导出个人资料到 SciVal

了解 Scopus 个人资料的更多信息



Marc T.M. Koper


386 文献

查看 Mendeley 个人资料

# 文献获取-他人推荐

H.H. Heenen, J.A. Gauthier, H.H. Kristoffersen, T. Ludwig, and K. Chan, J. Chem. Phys. **152**, 144703 (2020).

Google Scholar

☒ Articles ☐ Case law

# 文献获取-已有文献拓展

## References

- [1] M. Pumera, Graphene-based nanomaterials for energy storage, *Energy Environ. Sci.* 4 (2011) 668–674, <https://doi.org/10.1039/C0EE00295J>.
- [2] N. Choi, Z. Chen, S.A. Freunberger, X. Ji, Y. Sun, K. Amine, G. Yushin, L.F. Nazar, J. Cho, P.G. Bruce, Challenges facing lithium batteries and electrical double-layer capacitors, *Angew. Chem.* 51 (2012) 9994–10024, <https://doi.org/10.1002/anie.201201429>.
- [3] F. Shen, X. Chen, P. Gao, G. Chen, Electrochemical removal of fluoride ions from industrial wastewater, *Chem. Eng. Sci.* 58 (2003) 987–993, [https://doi.org/10.1016/S0009-2509\(02\)00639-5](https://doi.org/10.1016/S0009-2509(02)00639-5).
- [4] G. Chen, Electrochemical technologies in wastewater treatment, *Separ. Purif. Technol.* 38 (2004) 11–41, <https://doi.org/10.1016/j.seppur.2003.10.006>.
- [5] Y. Yavuz, A.S. Koparal, U.B. Ogutveren, Treatment of petroleum refinery wastewater by electrochemical methods, *Desalination* 258 (2010) 201–205, <https://doi.org/10.1016/j.desal.2010.03.013>.
- [6] N.R. Council, *Research Opportunities in Corrosion Science and Engineering*, The National Academies Press, Washington, DC, 2011 <https://doi.org/10.17226/13032>.
- [7] Y. Liu, D. Gokcen, U. Bertocci, T.P. Moffat, Self-terminating growth of platinum films by electrochemical deposition, *Science* 338 (6112) (2012) 1327–1330, <https://doi.org/10.1126/science.1228925>.
- [8] K.T. Butler, G.S. Gautam, P. Canepa, Designing interfaces in energy materials applications with first-principles calculations, *npj Comput. Mater.* 5 (2019), <https://doi.org/10.1038/s41524-019-0160-9>.



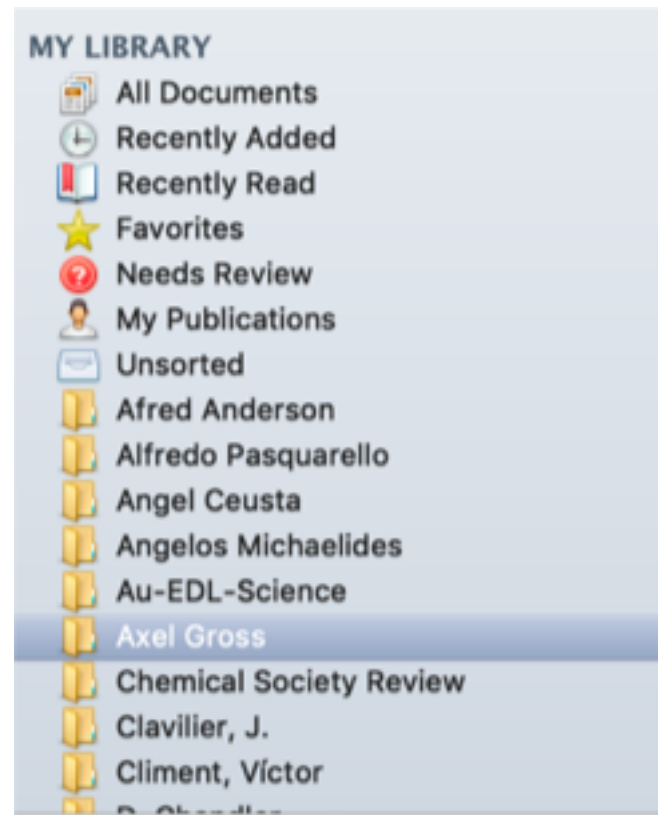
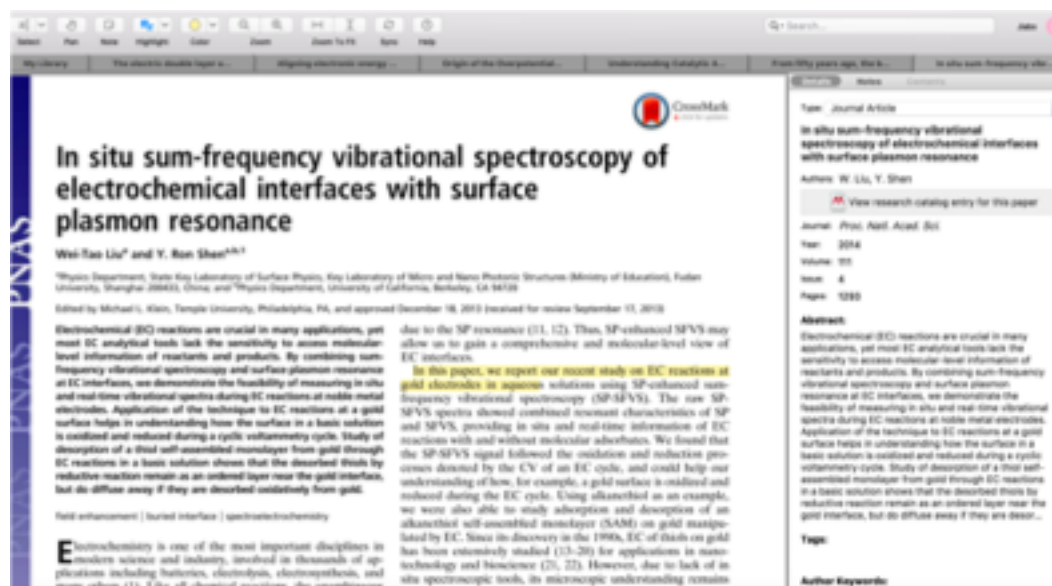
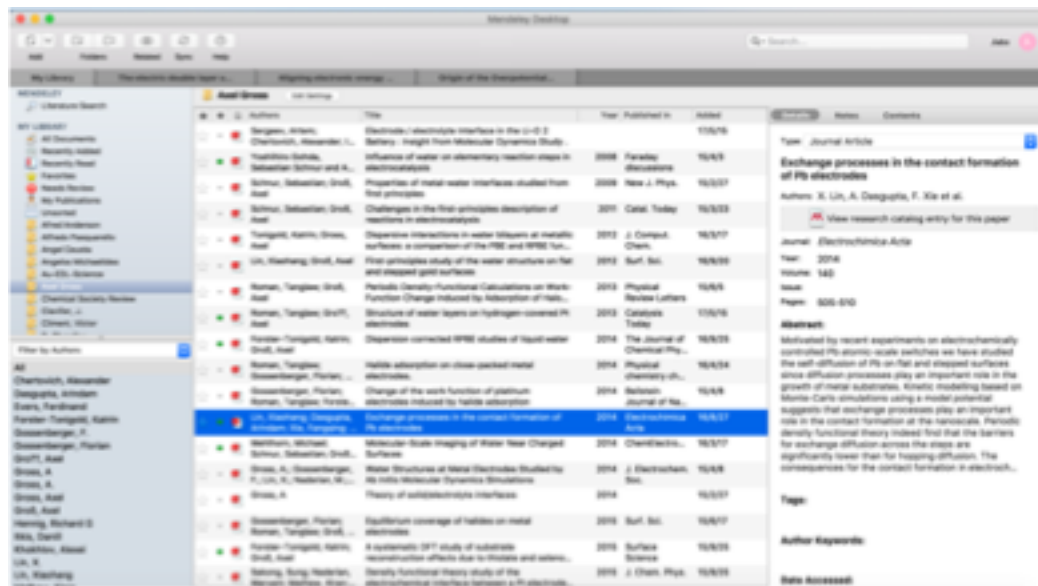
# 其它

- 研之成理
- 材料人
- X-MOL
- 蔻享学术(学术报告视频)
- <http://gen.lib.rus.ec/> (英文专著)
- Sci-hub.tw (英文文献)

# 文献管理

- 整理文献
- 方便使用
- 引用和输出

# 文献管理器-Mendeley



## Catalog IDs

ArXiv ID:

DOI: 10.1016/j.jelechem.2017.09.002

ISSN: 15726657

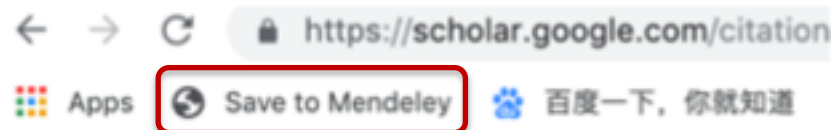
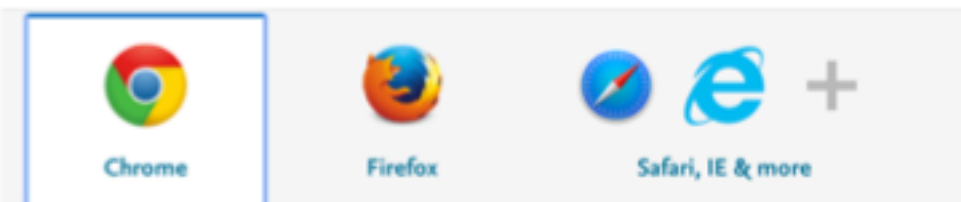
PMID:

Files:

Le, Cuesta, Cheng - 2018 - The structure of metal...

Add File...

# 文献管理器-Mendeley



1. Install the browser extension from the Chrome Web Store

Install Chrome browser extension



2. Save articles from supported sites

Click the extension button to the right of the address bar to save an article and retrieve its PDF full text (where available).

注册账号，便于文献在多个device上转移

[https://www.mendeley.com/reference-management/web-importer#id\\_1](https://www.mendeley.com/reference-management/web-importer#id_1)

# 文献管理器-其它

- EndNote
- Papers3/Readcube
- Zotero

达到主要目的为主，方便**使用**和**引用**（Word 和 Latex）

# 文献阅读

- 粗读
- 精读
- 拓展阅读

# 粗读文献-Title & Journal

基本检索 被引参考文献检索 高级检索

CO2 reduction  标题  检索 检索提示

+ 添加行 | 重设

时间跨度  
所有年份 (1950 - 2020) 

更多设置 

排序方式: 日期  被引频次 使用次数 相关性 更多 

1 / 651  

☐ 选择页面  导出... 添加到标记结果列表

 分析检索结果  
 创建引文报告

☐ 1. Optimizing electricity mix for CO2 emissions reduction: A robust input-output linear programming model  
作者: Kang, Jidong; Ng, Tsan Sheng; Su, Bin  
EUROPEAN JOURNAL OF OPERATIONAL RESEARCH 卷: 287 期: 1 页: 280-292 出版年: NOV 16 2020  
被引频次: 0 (来自所有数据库)  
使用次数 

 出版商处的全文 查看摘要 

Ethylene Selectivity in Electrocatalytic CO2 Reduction on Cu Nanomaterials: A Crystal Phase-Dependent Study

作者: Chen, Ye; Fan, Zhanxi; Wang, Jiong; 等.

JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 卷: 142 期: 29 页: 12760-12766 出版年: JUL 22 2020

# 粗读文献-Journal

- 综合类: Nature, Science, 大子刊, Nature communication, PNAS,
- 化学类: JACS, Angew. Chem. Int. Ed., ACS Catalysis
- 物理化学: JPC系列, PCCP, JCP
- 电化学: Electrochimica Acta, Electrochemical communication
- 其它相关



# 文献阅读-文献组成

## 粗读

- Title
- Abstract
- Figures and Tables
- Introduction
- Conclusion

## 精读

- Methods
- Results and Discussion
- Reference
- Support Information
- Authors (& affiliation)

# 粗读文献-开始阅读

## Insight into the Microenvironments of the Metal–Ionic Liquid Interface during Electrochemical CO<sub>2</sub> Reduction

Hyung-Kyu Lim,<sup>†</sup> Youngkook Kwon,<sup>‡,§</sup> Han Seul Kim,<sup>||</sup> Jiwon Jeon,<sup>||</sup> Yong-Hoon Kim,<sup>||</sup> Jung-Ae Lim,<sup>‡</sup> Beom-Sik Kim,<sup>‡,§</sup> Jina Choi,<sup>\*,‡</sup> and Hyungjun Kim<sup>\*,||,⊥</sup>

<sup>†</sup>Department of Chemical Engineering, Kangwon National University, Chuncheon, Gangwon-do 24341, Republic of Korea

<sup>‡</sup>Carbon Resource Institute, Korea Research Institute of Chemical Technology, 141 Gajeong-ro, Yuseong-gu, Daejeon 34114, Republic of Korea

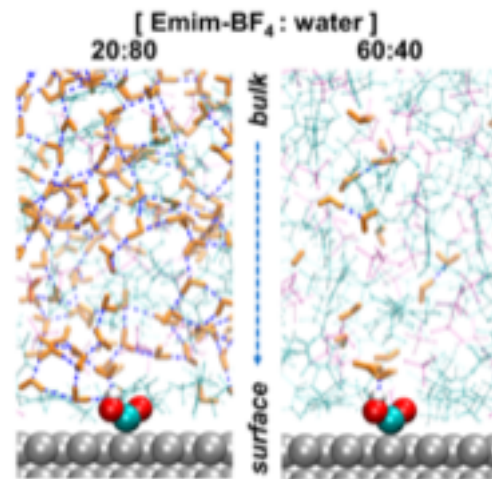
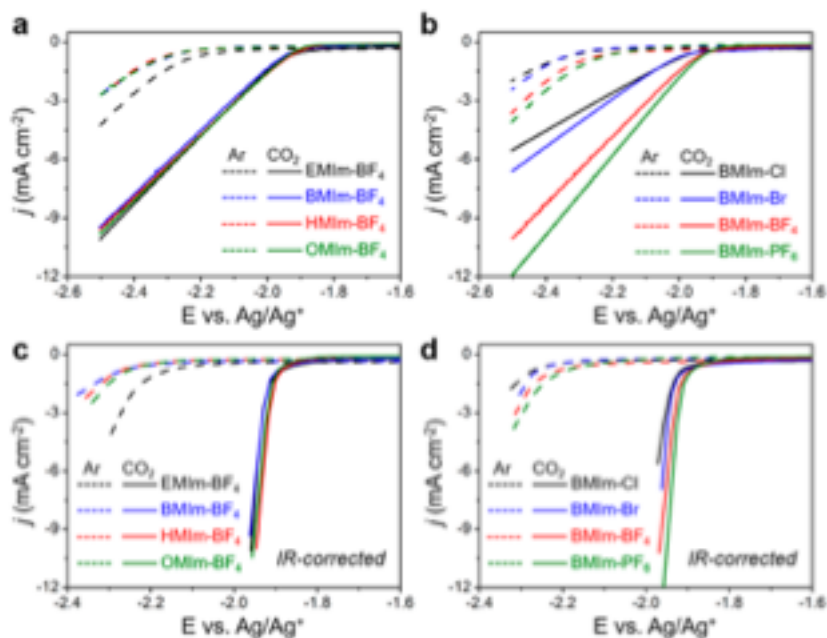
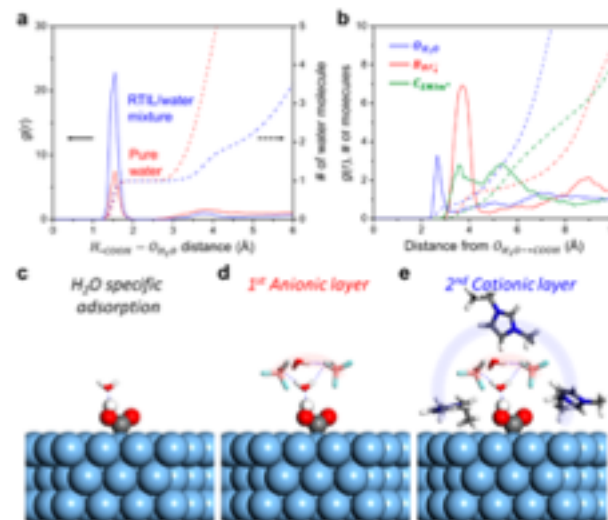
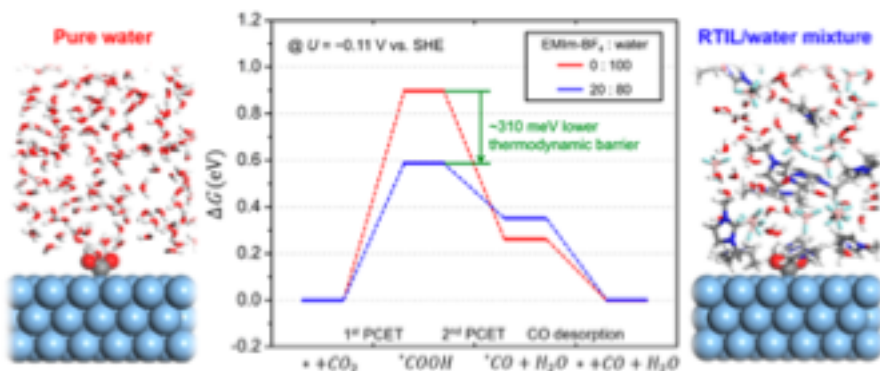
<sup>§</sup>Advanced Materials and Chemical Engineering, University of Science & Technology, 217 Gajeong-ro, Yuseong-gu, Daejeon 34113, Republic of Korea

<sup>||</sup>Graduate School of EEWS, Korea Advanced Institute of Science and Technology, 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Republic of Korea

<sup>⊥</sup>Department of Chemistry, Korea Advanced Institute of Science and Technology, 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Republic of Korea

<sup>S</sup> Supporting Information

# 粗读文献-Figures/Tables

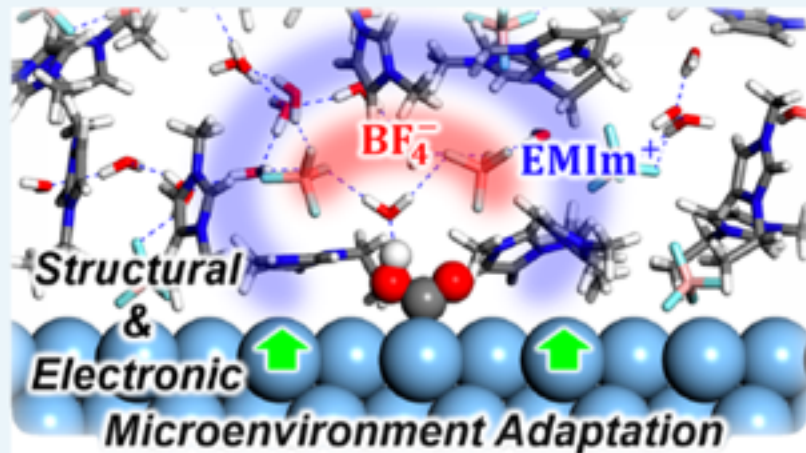


✓ 从图像与表格中看与你的研究是否相关

# 粗读文献-Abstract

**ABSTRACT:** Recently, many experimental and theoretical efforts are being intensified to develop high-performance catalysts for electrochemical CO<sub>2</sub> conversion. Beyond the catalyst material screening, it is also critical to optimize the surrounding reaction medium. From vast experiments, inclusion of room-temperature ionic liquid (RTIL) in the electrolyte is found to be beneficial for CO<sub>2</sub> conversion; however, there is no unified picture of the role of RTIL, prohibiting further optimization of the reaction medium. Using a state-of-the-art multiscale simulation, we here unveil the atomic origin of the catalytic promotion effect of RTIL during CO<sub>2</sub> conversion. Unlike the conventional belief, which assumes a specific intermolecular coordination by the RTIL component, we find that the promotion effect is collectively manifested by tuning the reaction microenvironment. This mechanism suggests the critical importance of the bulk properties (e.g., resistance, gas solubility and diffusivity, viscosity, etc.) over the detailed chemical variations of the RTIL components in designing the optimal electrolyte components, which is further supported by our experiments. This fundamental understanding of complex electrochemical interfaces will help in the development of more advanced electrochemical CO<sub>2</sub> conversion catalytic systems in the future.

**KEYWORDS:** *reaction mechanism, electrocatalysis, ionic liquids, multiscale simulation, solid–liquid interface*



✓ 从关键词和简介中推断研究内容与结论

# 粗读文献-Conclusions

## ■ CONCLUSION

On the basis of the atomistic details elucidated from our state-of-the-art simulations and systematic experiments, the catalytic promotion effect of RTILs is manifested by the collective participation of both cations and anions of RTILs. The RTIL at the EDL interface provides a suitable microenvironment for solvating the intermediate, which can be well preserved over the variations in chemical details because the solvation energy is dominated by the nonspecific interaction. We further anticipate that our comprehensive study of the nature of the complex electrochemical interface will be useful for designing enhanced electrochemical CO<sub>2</sub> reduction systems in the future. For example, the bulk properties of the reaction medium, such as the electrical resistance, gas solubility, gas diffusivity, and viscosity, are more critically optimized than a specific interaction pair. In addition, a certain amount of water is indispensable in facilitating the proton transfer by developing a percolated hydrogen bond network and improving the mass transport of RTIL components (Table S6) by screening the strong interionic electrostatic interaction.<sup>36</sup>

✓ 查看研究  
结果是否  
感兴趣



# 精读文献-Introduction背景

## ■ INTRODUCTION

There have been various technical explorations of the sustainable future of the global carbon-based economy. The development of CO<sub>2</sub> conversion technologies is imperative to successfully recycle the anthropogenically emitted greenhouse gas to produce future carbon resources of fuels and chemicals. Electrochemical CO<sub>2</sub> conversion is considered one of the most feasible and promising technologies because of its high reactivity under ambient conditions, its wide product window according to the type of catalyst, and its applicability in commercial processes. Thus, many experimental and theoretical studies have extensively developed high-performance electrochemical catalyst systems for CO<sub>2</sub> conversion to achieve a minimized overpotential, improved product selectivity, improved stability, etc.<sup>1–4</sup>

Beyond many efforts to optimize the catalyst material,<sup>5–7</sup> there was an interesting report in 2011 by Rosen et al.<sup>8</sup> They

showed that the activity of the electrochemical CO<sub>2</sub>-to-CO conversion reaction can be remarkably enhanced by an electrolyte mixture of 18 mol% 1-ethyl-3-methylimidazolium tetrafluoroborate (EMIm-BF<sub>4</sub>), one of the room-temperature ionic liquids (RTILs), and 82 mol % water. After this seminal work, many experimental reports have shown that the addition of RTIL to an electrolyte generally promotes the CO<sub>2</sub> reduction activity regardless of the choice of catalyst material (Ag, Au, or Pt).<sup>9,10</sup> Because the electrochemical catalytic reaction is manifested by the interfacial chemistry, which occurs at the heterogeneous interface between the catalyst surface and the liquid medium, this study successfully demonstrated the importance of a particular design of the reaction medium.

---

Received: November 6, 2017

Revised: January 5, 2018

Published: February 6, 2018

## ■ REFERENCES

- (1) Ganesh, I. Conversion of Carbon Dioxide into Methanol - a Potential Liquid Fuel: Fundamental Challenges and Opportunities (a Review). *Renewable Sustainable Energy Rev.* **2014**, *31*, 221–257.
- (2) Jhong, H. R.; Ma, S. C.; Kenis, P. J. A. Electrochemical Conversion of CO<sub>2</sub> to Useful Chemicals: Current Status, Remaining Challenges, and Future Opportunities. *Curr. Opin. Chem. Eng.* **2013**, *2*, 191–199.
- (3) Oloman, C.; Li, H. Electrochemical Processing of Carbon Dioxide. *ChemSusChem* **2008**, *1*, 385–391.

(19) Lim, H. K.; Lee, H.; Kim, H. A Seamless Grid-Based Interface for Mean-Field QM/MM Coupled with Efficient Solvation Free Energy Calculations. *J. Chem. Theory Comput.* **2016**, *12*, 5088–5099.

(20) Nakano, H.; Yamamoto, T. Accurate and Efficient Treatment of Continuous Solute Charge Density in the Mean-Field QM/MM Free Energy Calculation. *J. Chem. Theory Comput.* **2013**, *9*, 188–203.

(21) Lin, S. T.; Blanco, M.; Goddard, W. A. The Two-Phase Model for Calculating Thermodynamic Properties of Liquids from Molecular Dynamics: Validation for the Phase Diagram of Lennard-Jones Fluids. *J. Chem. Phys.* **2003**, *119*, 11792–11805.

✓ 较为全面得了解这个领域

# 精读文献-Introduction科学问题

However, there is little understanding of how RTIL participates in and promotes  $\text{CO}_2$  reduction chemistry, which limits further the systematic design of the catalyst system. Rosen et al. attributed the improved reactivity to a greater proton availability by the hydrolysis of  $\text{BF}_4^-$ <sup>11</sup> and a layer of  $\text{EMIm}^+$  on the catalyst surface<sup>12</sup> from follow-up experimental studies. In addition, the imidazole cation may directly chemically react with  $\text{CO}_2$  and serve as a proton donor, which promotes the proton-coupled electron transfer (PCET) process.<sup>13,14</sup> However, a recent experimental study has shown that methylation at the C2 position of imidazole promotes the  $\text{CO}_2$  reduction activity, which excludes the possibility of the direct catalytic role of a proton at the C2 position.<sup>15</sup> The experimental screening approach to identify the catalytic role of RTIL mostly relies on investigating the correlation between the catalytic activity and the chemical modifications of the RTIL.<sup>15,16</sup> Although this approach certainly provides valuable information about how the RTIL participates in the reaction, the concurrent change in the bulk properties of the RTIL after the chemical modifications adds many complications in deciphering the experimental observations. For example, methylation at the C2 position of 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ( $\text{EMIm-TFSI}$ ) increases the melting temperature from  $-14.7$  to  $22.0$  °C and changes the viscosity from 21 to 74 mPa s.<sup>17</sup> As summarized in our recent review,<sup>18</sup> there have been various efforts to identify mechanisms through various experimental and theoretical studies, but no decisive conclusion has been drawn.

➤ 作者总结的领域内关键科学问题

## 具体解决方法-最后一段

In this study, we unveil the atomic origin of the catalytic promotion effect of RTILs during electrochemical  $\text{CO}_2$  conversion by means of the first-principles-based multiscale simulation method (DFT-CES). In contrast to the previous conception that a certain type of direct chemical interaction between the RTIL component and the reaction intermediate promotes catalytic activity (which has often been assumed in the interpretation of experimental results), we find that RTIL components participate in the reaction in a collective manner by adjusting the reaction microenvironment during  $\text{CO}_2$  reduction. On the basis of our mechanism, we designed and performed a series of systematic experiments. This demonstrates the importance of bulk properties such as a bulk conductivity to the detailed chemical interactions of RTIL, suggesting a new design guideline for the reaction medium to enhance  $\text{CO}_2$  reduction.

# 精读文献-Methods

## ■ METHODS

**Multiscale Simulation Method (DFT-CES).** To briefly explain the key aspects of the DFT-CES method for the

**Computational Details.** First, we built four types of solvent models with different molar ratios of EMIm-BF<sub>4</sub> to water: from pure water (0:100) to pure ionic liquid (100:0) (Table S1). We used the LAMMPS (Large-scale Atomic/

**Electrochemical Measurements.** Electrochemical experiments were performed in a three-electrode system. A silver foil (Alfa Aker, 99.998%) was polished before each measurement

✓ 厘清所用方法，根据自己的研究目的决定理解程度。



# 精读文献-Results and Discussion

- 线性讲述
- 段内第一句
- 结合图表快速定位
- Support Information

## ■ RESULTS AND DISCUSSION

**Reaction Thermodynamics.** Using the DFT-CES/2PT method, we investigate the reaction thermodynamics for the CO<sub>2</sub>-to-CO reduction on the Ag(111) surface when the electrolyte phase is water or an EMIm-BF<sub>4</sub>/water mixture (20:80 molar ratio). The simulation cell in [Figure S1](#) includes

**Water Molecule Coordinating \*COOH.** Surprisingly, we find that the local coordinating environment of \*COOH is

**Collective Change in the Reaction Microenvironment.** Beyond the comparison of the direct coordinating environ-

## 4. RESULTS AND DISCUSSION

**4.1. Convergence of SCRF Iterations.** To check the convergence of DFT-CES, we monitored how  $E_{\text{reorg}}$  from DFT calculations changed over the SCRF iterations. As shown in

**4.2. Reaction Field Sampled from MD.** After running enough SCRF iterations to converge  $E_{\text{reorg}}$ , we visualized the reaction field of  $\langle \rho_{\text{solvent}} \rangle$  in [Figure 3](#) for two representative

# 精读文献- Authors

## Insight into the Microenvironments of the Metal–Ionic Liquid Interface during Electrochemical CO<sub>2</sub> Reduction

Hyung-Kyu Lim,<sup>†,‡</sup> Youngkook Kwon,<sup>‡,§</sup> Han Seul Kim,<sup>||</sup> Jiwon Jeon,<sup>||</sup> Yong-Hoon Kim,<sup>||,‡</sup> Jung-Ae Lim,<sup>‡</sup> Beom-Sik Kim,<sup>‡,§</sup> Jina Choi,<sup>\*,‡</sup> and Hyungjun Kim<sup>\*,||,1,‡</sup>

### ■ AUTHOR INFORMATION

#### Corresponding Authors

\*Phone: +82-42-860-7396. E-mail: [jchoi@krikt.re.kr](mailto:jchoi@krikt.re.kr).

\*Phone: +82-42-350-1725. E-mail: [linus16@kaist.ac.kr](mailto:linus16@kaist.ac.kr).

### ■ REFERENCES

(18) Lim, H.-K.; Kim, H. The Mechanism of Room-Temperature Ionic-Liquid-Based Electrochemical CO<sub>2</sub> Reduction: A Review. *Molecules* **2017**, *22*, 536.

(19) Lim, H. K.; Lee, H.; Kim, H. A Seamless Grid-Based Interface for Mean-Field QM/MM Coupled with Efficient Solvation Free Energy Calculations. *J. Chem. Theory Comput.* **2016**, *12*, 5088–5099.

(36) Jeon, J.; Kim, H.; Goddard, W. A.; Pascal, T. A.; Lee, G. I.; Kang, J. K. The Role of Confined Water in Ionic Liquid Electrolytes for Dye-Sensitized Solar Cells. *J. Phys. Chem. Lett.* **2012**, *3*, 556–559.

# 文献阅读

- ✓ 大部分文献粗读，少量精度（保证文章阅读量）；
- ✓ 建议一篇文献一次性看完，即使有很多不懂的地方；
- ✓ 结合自己的数据，隔断时间多次阅读核心的文献，可获得灵感；
- ✓ 通过多种工具，跟踪最新的文献；
- ✓ 定期进行文献总结，综述，厘清目前研究的不足之处及我们可弥补的地方。

## SHARE



4K



1



CREDIT: N. HENDRICKSON / ISTOCKPHOTO

## How to read a scientific paper

By [Adam Ruben](#) | Jan. 20, 2016, 3:15 PM

## FOLLOW SCIENCE CAREERS



### Search Jobs

Enter keywords, locations or job types to start searching for your new science career.

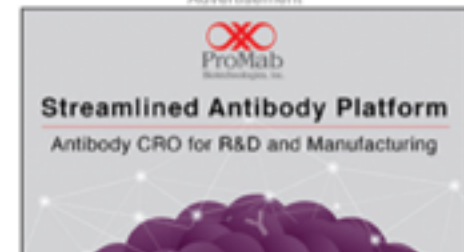
[Register](#) [Advanced Search](#)

Advertisement



### Streamlined Antibody Platform

Antibody CRO for R&amp;D and Manufacturing



Nothing makes you feel stupid quite like reading a scientific journal article.