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上海大学

博士学位论文

SHANGHAI UNIVERSITY
DOCTORAL DISSERTATION

题目	基于小数据机器学习方法的材料设计研究

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附录

表 S1 常用的文本挖掘软件与平台
Table S1 Commonly used software and platform of text mining

名称	简介	链接
ActivePoint	提供自然语言处理与智能在线目录，基于上下文搜索与 ActivePoint 的 TX5(TM)发现引擎	http://www.activepoint.com/
Basis Technology	为分析非结构化多语种文本提供自然语言处理技术	https://www.basistech.com/
Copernic Summarizer	能从不同的应用程序中阅读和总结文档和网页的文本内容	https://copernic.com/en/
DiscoverText	基于云端的文本分析解决方案，拥有许多强大的功能，包括一个主动学习机器的分类引擎	https://discovertext.com/
IBM SPSS Predictive Analytics	用于数据和文本挖掘的套件	https://www.ibm.com/spss
ISYS Search Software	一个专注于嵌入式搜索、文本提取、联合访问解决方案和文本分析的企业搜索软件供应商	https://www.hyland.com/en/perceptive
KNIME	一个开源的分析平台，为当前的文本分析软件提供扩展，包括了 Stanford NLP、Palladin 和 Linguamatics	https://www.knime.com/
Lexalytics	提供企业级和可托管文本的分析软件，可将非结构化文本转换成结构化数据	https://www.lexalytics.com/
Megaputer Text Analyst	提供自由格式文本的语义分析、汇总、聚类、导航和包含搜索动态聚焦的自然语言检索	https://www.megaputer.com/
MonkeyLearn	可创建机器学习应用程序的文本挖掘工具。根据你所支付的价格，它能够通过 web 和 API 提供分类、提取、集群和回归模块	https://monkeylearn.com/
Ontotext	通过语义技术的混合文本挖掘、推理和图形数据库提供优化的知识管理、搜索和语义的分析解决方案	https://www.ontotext.com/

名称	简介	链接
VP Student Edition	强大的文本挖掘和可视化工具，用于从科学文献和其他字段结构化文本数据库中发现知识	https://vpinstitute.org/vp-marketplace/
Aika	一种用于文本频繁挖掘模式的开源库，使用了神经网络和语法归纳的思想	http://aika.network/
Coding Analysis Toolkit (CAT)	免费、开源、基于 web 的文本分析工具	http://cat.texifter.com/

表 S2 材料数据库及其简介

Table S2 Materials databases and corresponding introduction

名称	简介	ULR
Materials Project	提供 130,000 多种无机化合物的结构信息和性质，包括能带结构、弹性张量、压电张量和第一原理计算性质	https://www.materialsproject.org/
OQMD	OQMD 是一个基于密度泛函理论的计算热力学和结构数据库。数据库中的材料包括电池材料、储氢材料、太阳能材料和热电材料。	http://oqmd.org/
NIST	NIST 数据库是一个全面的质谱数据库，可用于基于 LC-MS 代谢组学的代谢物鉴定，几乎涵盖所有材料系统	https://www.nist.gov/srd/
ICSD	ICSD 自 1913 年出版以来，已收录近 10 万种化合物。该数据库包括化学式、单胞参数、空间群、原子坐标热参数和其他信息。	http://icsd.fiz-karlsruhe.de/
MPDS	MPDS 是世界上最全面的无机材料数据库。该数据库收录了 1900 年至今世界各地发表的材料文献，收集了 100 多万条实验和计算数据。MPDS 涵盖的材料特性包括力学、热力学、电磁学、光学等。	https://asm.mpds.io
NOMAD	NOMAD 建立了一个综合数据库，专门用于收集所有计算材料数据，目前已收录了数百万个计算结果，供公开使用	https://nomad-coe.eu
AFLOWlib	AFLOWlib 存储了超过 356 万种材料结构，包括无机化合物、二元合金和多组分合金，以及 7 亿条第一原理计算的材料属性数据，是众多数据库中数据量最大的。	http://aflowlib.org/
材料基因工程数据库	中国最大的材料基因工程数据库平台。除数据库外，该平台还拥有第一原理在线计算引擎、原子势函数库、在线数据挖掘系统等多项功能	https://www.mgedata.cn/

名称	简介	ULR
OMDB	OMDB 是一个三维有机晶体电子结构数据库，包含迄今已知的纯有机化合物和有机金属化合物的电子结构、状态密度和其他特性。	http://omdb.diracmaterials.org
CSD	CSD 于 1965 年创建的小分子有机化合物和金属有机化合物晶体结构数据库。该数据库包括来自文献的 115 万个小分子有机化合物和金属有机化合物的晶体结构数据，包括单胞参数、原子坐标等。	https://www.ccdc.cam.ac.uk/
QM9	QM9 为相关、一致和全面的有机小分子化学空间提供了量子化学性质。	https://paperswithcode.com/data et/qm9
High entropy alloy database	TCHEA6 是专为高熵合金 (HEA) 而设计的热力学和属性数据库	https://thermocalc.com/products/databases/high-entropy-alloys/
Starrydata2	Starrydata2 可以从科学论文的制图中自动提取数值数据和相应样品的化学成分，并已成功地从制图图像中收集了超过 11,500 个热电材料样品的实验数据。	https://www.Starrydata2.org/
Novamag databse	为磁性化合物和磁性团簇提供了大量数据集，重点关注无稀土磁体。可用数据集包括 (i) 晶体学数据、(ii) 热力学性质和 (iii) 磁性能。	https://www.novomag.physics.iastate.edu/structure-database
AtomWork-Adv	无机材料数据库，包括晶体结构、材料特性、相图、出版物、X 射线衍射。	https://atomworkadv.nims.go.jp/
Bradley Melting Point Database	让-克劳德-布拉德利（Jean-Claude Bradley）的开放熔点数据集，包括 28,645 次测量。	https://figshare.com/articles/dataset/Jean_Claude_Bradley_Open_Melting_Point_Datset/103167
FeeSolv	The Free Solvation (FreeSolv)数据库提供小分子在水中的实验和计算水合自由能	https://github.com/MobleyLab/FreeSolv
PubChem	PubChem 是全球最大的免费化学信息库。通过名称、分子式、结构和其他标识符搜索化学品。查找化学和物理性质、生物活性、安全性和毒性信息、专利、文献引用等。	https://pubchem.ncbi.nlm.nih.gov/
Pauling file	The Pauling file 收集了从 1900 年至今 35,000 多份出版物中的无机材料数据，其中包括 350,000 个晶体结构、50,000 个相图和 150,000 个物	https://www.paulingfile.com/

名称	简介	ULR
	理性质。	
PoLyInfo	PoLyInfo 提供了有关数百种聚合物材料的化学结构、特性和合成方法的信息	https://polymer.nims.go.jp/
Materials Cloud	Materials Cloud 是一个开放式材料科学平台，旨在实现计算材料科学资源的无缝共享和传播，提供教育、研究、模拟软件和经过整理的原始数据	https://www.materialscloud.org

表 S3 材料科学中的高通量计算工具包

Table S3 Toolkits of high-throughput computation in materials science

名称	简介	DFT 软件交互
MatCloud	MatCloud 是一个集成了高通量计算和材料数据库的平台	VASP
AFLOW	AFLOW 是杜克大学开发的一个自动化高通量计算材料发现框架，可用于对合金、无机晶体结构和其他材料的特性进行高通量计算。	VASP, QE
FireWorks	FireWorks 是一款用于高通量计算任务的开源软件，已在计算化学和材料领域完成了数百万次高通量计算任务。	VASP
JARVIS	JARVIS 是一个数据驱动的材料设计工具包，集成了材料的 DFT 计算特性、力场计算数据库、机器学习预测特性数据库以及相关的高通量计算和机器学习工具。	VASP, QE, BolzTrap, LAMMPS, WIEN2K
ASE	ASE 是一个用 Python 语言编写的软件包，可轻松计算材料属性和完成其他高通量计算模拟任务。	VASP, QE, CASTEP
AiiDA	AiiDA 是一个开源的高通量计算框架，集成了计算和相关数据任务的自动化、管理、存储、共享和复制功能。	QE
SEHC	SEHC 是一款具有自我评估筛选功能的高通量计算软件包。SEHC 通过评估高通量计算任务的合理性，提前中断不合理的高通量计算任务，从而提高高通量计算的效率。	VASP
JAMIP	JAMIP 是一款大型计算材料设计软件包，集高通量计算、数据生成、收集、管理和存储以及机器学习于一体。	VASP
Pymatgen	Pymatgen 为大量第一原理 DFT 计算软件（如 VASP、ABINIT 和 Gaussian）提供应用编程接口，支持各种格式的材料文件。	VASP, ABINIT, Gaussian

名称	简介	DFT 软件交互
RadonPy	RadonPy 是一个开放源码 Python 库，用于全原子经典分子动力学模拟的全自动聚合物特性计算，它已成功对 1000 多种具有各种热物理性质的无定形聚合物进行了高通量计算	LAMMPS

表 S4 常用的高通量制备与表征技术

Table S4 Commonly used high-throughput preparation and characterization techniques

方法	制备/ 表征	简介
扩散多节点法	制备	扩散多节点法是一种高通量制备方法，通过在一定成分范围内利用扩散作用形成二元和三元扩散节点，从而在一定温度下形成以预定方式排列且成分不断变化的多种块状金属。
共沉积法	制备	共沉积方法利用各沉积源与基底相对角度和位置的变化，在同一基底上沉积多种合金成分，形成合金成分梯度分布的材料样品。
连续掩膜法	制备	连续掩膜法是通过控制基底阶段来控制样品的沉积速率，然后利用涂层和时移掩膜技术形成成分可控的多组分合金复合样品
离散掩膜法	制备	离散掩膜法是将涂层技术和掩膜技术相结合，利用连续掩膜获得不同离散组分样品的方法，适用于制备多组分、组分空间跨度大的新材料。
喷射合成法	制备	喷射合成法是通过喷射技术将不同组分的原材料沉积在基底或反应腔中，从而获得多组分复合材料样品。
微流控技术	制备	微流控技术是一种利用微通道精确控制微尺度流体的制备技术。该技术的主要平台是微流控芯片，可集成到样品制备和表征等基本操作中。
材料基因组合芯片	制备	材料基因组合芯片技术是将离散的样品以阵列的形式集成到样品库或反应库中，利用组合理论的思想和理论，通过各种反应物或前体化合物的各种化学反应，快速高效地制备出大量样品。
强引力场沉积原子法	制备	由于不同元素的相对原子质量不同，在强离心和加热的作用下，材料中各成分所受的离心力也不同，因此可以利用强引力场将均质材料逐渐转化为具有成分梯度的材料
同步辐射源	表征	同步辐射源可在整个光谱范围内实现高亮度微聚焦，从而提高高通量表征所需的光通密度、亮度和分辨率。

方法	制备/ 表征	简介
同步辐射源	表征	溅射中子源配备了一个光谱仪，可以测量高通量样品的能量和动力学特性 以准确捕捉物质的整体特性
数字三维微观结构表征	表征	数字三维微观结构表征是通过机械抛光技术获得二维图像，然后利用计算机将二维图像处理成数字三维结构。
时域热反射技术	表征	时域热反射技术可以快速测量激光反射率与样品表面温度的时间关系。
纳米压头	表征	纳米压头可表征纳米级材料的强度、硬度、弹性模量和其他机械性能。
扫描探针显微镜	表征	扫描探针显微镜适用于高通量材料结构和表面微区的定性分析和表征，可生成高分辨率图像
Evanescent 微波探针显微镜	表征	Evanescent 微波探针显微镜具有极高的微区分辨率和精确的数据采集系统，可用于对材料芯片的电磁特性进行高通量表征。
平行纳米扫描量热仪	表征	平行纳米扫描量热仪装置由一系列微加热或量热单元基板组成，可同时测量焓变、热容量、相变温度等热力学参数。

表 S5 常用的不平衡学习方法

Table S5 Commonly used imbalanced learning methods

方法	技术基础	简介
RUS	抽样	随机抽取多数类样本，并将其从数据集中移除，直到达到理想的类分布为止
RUSBoost	RUS/ Boosting	RUSBoost 采用随机欠采样技术，在 AdaBoost.M2 的每次迭代中移除多数类中的实例，使新的欠采样数据集中的实例权重正常化。
NUS	KNN	NUS 将欠采样技术与噪声过滤技术相结合，过滤掉原始少数群体数据集中的噪声数据，然后使用新的数值数据集训练分类器
DBU	KNN	DBU 根据样本的相似系数选择一定数量的样本作为多数类数据的重采样。对于少数类样本，则通过删除相似性系数为 0 的示例来消除噪声，从而达到对数据进行采样和调整不平衡现象的目的。
Tomek Links	抽样	两个不同类别的样本被定义为一对 Tomek Link，噪声数据则通过第三个样本点距离约束去除
NCL	抽样	NCL 随机找到一定数量的邻近样本，通过对样本类别的判断，删除一定数量的多数类，而少数类则不做处理。

方法	技术基础	简介
SMOTE	SMOTE	SMOTE 通过随机抽取同类相邻样本进行插值，生成新的少数类样本，而不会重复
SMOTEENN	SMOTE	SMOTEENN 使用 SMOTE 生成新的少数群体样本，然后在获得扩展数据集后，使用 ENN 算法消除新数据集中的 Tomek Link。
KM-SMOTE	SMOTE/ K-means	KM SMOTE 首先使用 K-means 算法对少数类样本进行聚类，并将获得的聚类作为区域来执行 SMOTE 插值
Borderline-SMOTE	SMOTE	边界-SMOTE 与 SMOTE 的超采样技术相同，只是对少数群体的边界进行超采样
Safe-Level-SMOTE	SMOTE	安全等级-SMOTE 以不同的权重对少数实例进行仔细采样，在生成实例之前为每个正实例分配一个安全等级
DBSMOTE	SMOTE	DBSMOTE 沿着从每个阳性实例到少数类群伪中心点的最短路径生成样本
SMOTEBagging	SMOTE/ Bagging	SMOTEBagging 将 SMOTE 算法与袋集模型相结合，并对其进行扩展，以解决多类数据集问题，从而提高整体性能和多样性
SMOTEBoost	SMOTE/ Boosting	SMOTEBoost 在每次提升迭代中引入 SMOTE，以学习更广泛的少数类别决策区域
AEIRF	RF	通过混合抽样策略与随机森林的结合，AEIRF 不仅发挥了混合抽样能更全面地处理数据集的优势，还结合了随机森林平衡误差和抗过拟合能力强的优点。
ARIRF	RF	ARIRF 通过对随机森林中的每个子树采用混合采样策略，提高了基础分类器的多样性，并增强了分类器的效果
NOBDF	SVM	NOBDF 将超采样和 SVM 结合起来进行数据集重构，在正负分类准确率和整体分类性能方面都取得了良好的效果。
FSVMs	SVM	FSVM 将超采样方法与模糊半监督 SVM 学习方法相结合，在分割策略的基础上进一步解决多类不平衡问题
GAN	DL	利用 WGAN（Wasserstein GAN）对 GAN 的损失函数和网络结构进行适当修改，使其在训练中更加稳定。与用于数据增强实验的 SMOTE 相比，WGAN 对阈值的敏感度低于 SMOTE。
GAN-DAE	DL	GAN-DAE 通过生成器和判别器的对抗训练，获取不平衡数据中正负样本的特征，从而改善数据样本的不平衡性。
DNN	DL	DNN 提取少数样本的特征作为基本特征，然后添加一些伪特征生成新样本，以弥补少数样本的不足，从而有效改善不平衡数据集的分类结果

方法	技术基础	简介
D -WELM	ELM	D-WELM 不仅考虑了样本类别数量的影响，还考虑了数据分布特征的影响，即数据的分散程度
CHMDT	DT	CHMDT 用于不平衡数据集的二元分类，两类数据不平衡以提高分类精度
WBCRF	K-means	WBCRF 采用 K 均值聚类法进行欠采样，并选择误分类成本下降最大的属性进行划分。

表 S6 铁电/非铁电钙钛矿分类模型训练集

Table S6 Training data of the classification model

化学式	类别	化学式	类别
$BaCu_{0.33}Nb_{0.67}O_3$	0	$SrFe_{0.5}Ta_{0.5}O_3$	0
$SrCu_{0.33}Nb_{0.67}O_3$	0	$PbNi_{0.5}Ti_{0.25}W_{0.25}O_3$	0
$SrCu_{0.33}Ta_{0.67}O_3$	0	$PbMn_{0.5}Nb_{0.5}O_3$	0
$PbCd_{0.33}Nb_{0.67}O_3$	0	$Sr_{0.5}La_{0.5}Cu_{0.5}Sb_{0.5}O_3$	0
$BaBi_{0.5}Nb_{0.5}O_3$	0	$Sr_{0.5}La_{0.5}Cu_{0.33}Sb_{0.67}O_3$	0
$BaBi_{0.5}Ta_{0.5}O_3$	0	$Sr_{0.5}La_{0.5}Cu_{0.5}Ta_{0.5}O_3$	0
$TlNa_{0.2}W_{0.8}O_3$	0	$SrNi_{0.5}Re_{0.5}O_3$	0
$TlCd_{0.25}W_{0.75}O_3$	0	$SrFe_{0.5}Re_{0.5}O_3$	0
$TlY_{0.33}W_{0.67}O_3$	0	$PbMn_{0.5}W_{0.5}O_3$	1
$TlGd_{0.33}W_{0.67}O_3$	0	$PbMn_{0.5}Re_{0.5}O_3$	1
$TlDy_{0.33}W_{0.67}O_3$	0	$PbMn_{0.5}Re_{0.5}O_3$	1
$TlFe_{0.33}W_{0.67}O_3$	0	$PbMn_{0.5}W_{0.5}O_3$	1
$TlTi_{0.33}W_{0.67}O_3$	0	$PbCd_{0.5}W_{0.5}O_3$	1
$NaTaO_3$	0	$NaNbO_3$	1
$SrTiO_3$	0	$PbMg_{0.5}W_{0.5}O_3$	1
$BaTiO_3$	0	$PbCo_{0.5}W_{0.5}O_3$	1
$PbTiO_3$	0	$PbIn_{0.5}Nb_{0.5}O_3$	1
$PbSc_{0.5}Nb_{0.5}O_3$	0	$PbYb_{0.5}Nb_{0.5}O_3$	1
$PbSc_{0.5}Ta_{0.5}O_3$	0	$PbLu_{0.5}Nb_{0.5}O_3$	1
$PbFe_{0.5}Ta_{0.5}O_3$	0	$PbYb_{0.5}Ta_{0.5}O_3$	1
$PbZn_{0.33}Nb_{0.67}O_3$	0	$PbZn_{0.5}W_{0.5}O_3$	1
$PbCo_{0.33}Nb_{0.67}O_3$	0	$PbNi_{0.5}W_{0.5}O_3$	1
$PbNi_{0.33}Nb_{0.67}O_3$	0	$PbBi_{0.5}Nb_{0.5}O_3$	1
$PbMg_{0.33}Ta_{0.67}O_3$	0	$PbCd_{0.25}Mn_{0.25}Nb_{0.5}O_3$	1

化学式	类别	化学式	类别
$PbCo_{0.33}Ta_{0.67}O_3$	0	$PbCd_{0.25}Ti_{0.25}Ta_{0.5}O_3$	1
$PbNi_{0.33}Ta_{0.67}O_3$	0	$PbSnO_3$	1
$PbFe_{0.67}W_{0.33}O_3$	0	$PbZr_{0.94}Ti_{0.06}O_3$	1
$DyCrO_3$	0	$SrMn_{0.5}Re_{0.5}O_3$	1
$YbCrO_3$	0	$BaMn_{0.5}Re_{0.5}O_3$	1
$LuCrO_3$	0	$PbFe_{0.5}Re_{0.5}O_3$	1
$PrCrO_3$	0	$PbCo_{0.5}Re_{0.5}O_3$	1
$PbCo_{0.5}W_{0.5}O_3$	0	$PbNi_{0.5}Re_{0.5}O_3$	1
$CdFe_{0.5}Nb_{0.5}O_3$	0	$BaCd_{0.33}Nb_{0.67}O_3$	1
$CdSc_{0.5}Nb_{0.5}O_3$	0	$BaMg_{0.33}Nb_{0.67}O_3$	1
$CdMg_{0.33}Nb_{0.67}O_3$	0	$SrCd_{0.33}Nb_{0.67}O_3$	1
$PbCr_{0.5}Nb_{0.5}O_3$	0	$BaFe_{0.5}Nb_{0.5}O_3$	1
$PbLi_{0.25}Sc_{0.25}W_{0.5}O_3$	0	$BaSc_{0.5}Nb_{0.5}O_3$	1
$PbLi_{0.25}Fe_{0.25}W_{0.5}O_3$	0	$CaCr_{0.5}Nb_{0.5}O_3$	1
$PbLi_{0.25}In_{0.25}W_{0.5}O_3$	0	$NdMg_{0.5}Ti_{0.5}O_3$	1
$PbLi_{0.25}Tb_{0.25}W_{0.5}O_3$	0	$Na_{0.5}La_{0.5}TiO_3$	1
$PbLi_{0.25}Yb_{0.25}W_{0.5}O_3$	0	$K_{0.5}La_{0.5}TiO_3$	1
$PbLi_{0.25}Gd_{0.25}W_{0.5}O_3$	0	$Na_{0.5}Nd_{0.5}TiO_3$	1
$PbLi_{0.25}La_{0.25}W_{0.5}O_3$	0	$CdSnO_3$	1
$PbLi_{0.25}Sm_{0.25}W_{0.5}O_3$	0	$CaZrO_3$	1
$PbNa_{0.25}Y_{0.25}W_{0.5}O_3$	0	$CaSnO_3$	1
$PbCd_{0.45}Nb_{0.22}W_{0.33}O_3$	0	$CaMoO_3$	1
$PbSc_{0.25}Cr_{0.25}W_{0.5}O_3$	0	$CaRuO_3$	1
$PbMg_{0.25}Mn_{0.25}W_{0.5}O_3$	0	$CaTiO_3$	1
$PbCd_{0.25}Mn_{0.25}W_{0.5}O_3$	0	$CdPbO_3$	1
$PbCo_{0.25}Mn_{0.25}W_{0.5}O_3$	0	$CdZrO_3$	1
$PbNi_{0.25}Mn_{0.25}W_{0.5}O_3$	0	$SrPbO_3$	1
$PbNi_{0.25}Mn_{0.25}Nb_{0.5}O_3$	0	$SrSnO_3$	1
$PbCo_{0.25}Mn_{0.25}Nb_{0.5}O_3$	0	$SrZrO_3$	1
$PbMg_{0.25}Mn_{0.25}Nb_{0.5}O_3$	0	$BaSnO_3$	1
$PbZn_{0.25}Mn_{0.25}Nb_{0.5}O_3$	0	$BaSb_{0.5}In_{0.5}O_3$	1
$PbMg_{0.25}Mn_{0.25}Ta_{0.5}O_3$	0	$BaBiO_3$	1
$PbNa_{0.25}Sc_{0.25}W_{0.5}O_3$	0	$BaW_{0.5}Ba_{0.5}O_3$	1

化学式	类别	化学式	类别
$PbNa_{0.25}Dy_{0.25}W_{0.5}O_3$	0	$BaNi_{0.5}W_{0.5}O_3$	1
$PbFe_{0.5}Mn_{0.25}W_{0.25}O_3$	0	$BaZrO_3$	1

表 S7 铁电/非铁电钙钛矿分类模型测试集

Table S7 Testing data of the classification model

化学式	类别	化学式	类别
$BaW_{0.5}Cu_{0.5}O_3$	0	$PbNi_{0.25}Mn_{0.25}Ta_{0.5}O_3$	0
$SrW_{0.5}Cu_{0.5}O_3$	0	$PbLi_{0.25}Ni_{0.25}W_{0.5}O_3$	0
$BaCu_{0.33}Ta_{0.67}O_3$	0	$Sr_{0.5}La_{0.5}Cu_{0.5}Nb_{0.5}O_3$	0
$PbSc_{0.67}W_{0.33}O_3$	0	$SrCo_{0.5}Re_{0.5}O_3$	0
$BaBi_{0.67}W_{0.33}O_3$	0	$PbMn_{0.67}W_{0.33}O_3$	1
$TlMg_{0.25}W_{0.75}O_3$	0	$PbZrO_3$	1
$PbFe_{0.5}Nb_{0.5}O_3$	0	$PbLu_{0.5}Ta_{0.5}O_3$	1
$PbFe_{0.5}Nb_{0.5}O_3$	0	$PbGa_{0.5}Nb_{0.5}O_3$	1
$TlZr_{0.5}W_{0.5}O_3$	0	$PbCd_{0.33}Mn_{0.33}W_{0.34}O_3$	1
$CdCr_{0.5}Nb_{0.5}O_3$	0	$BaZn_{0.33}Nb_{0.67}O_3$	1
$PbLi_{0.25}Co_{0.25}W_{0.5}O_3$	0	$LaMg_{0.5}Ti_{0.5}O_3$	1
$PbLi_{0.25}Y_{0.25}W_{0.5}O_3$	0	$CaMnO_3$	1
$PbLi_{0.25}Pr_{0.25}W_{0.5}O_3$	0	$K_{0.5}Bi_{0.5}ZrO_3$	1
$PbLi_{0.33}Zr_{0.17}W_{0.5}O_3$	0	$SrMnO_3$	1
$PbSc_{0.56}Nb_{0.11}W_{0.33}O_3$	0		

表 S8 *SSA* 回归模型训练数据集

Table S8 Training data of the *SSA* regression model

化学式	*SSA*/ m^2g^{-1}	化学式	*SSA*/ m^2g^{-1}
$La_{0.9}Mg_{0.1}MnO_3$	37.1	$PrMn_{0.8}Ni_{0.2}O_3$	13.97
$LaMn_{0.9}Mg_{0.1}O_3$	24.8	$PrMn_{0.6}Ni_{0.4}O_3$	26.61
$LaFe_{0.975}Pd_{0.025}O_3$	22	$PrMn_{0.4}Ni_{0.6}O_3$	12.63
$LaFe_{0.95}Pd_{0.05}O_3$	27	$PrMn_{0.2}Ni_{0.8}O_3$	8.93
$LaCo_{0.1}Mn_{0.9}O_3$	57	$LaNi_{0.4}Fe_{0.6}O_3$	5.4
$LaCo_{0.2}Mn_{0.8}O_3$	56	$La_{0.9}Ce_{0.1}Ni_{0.4}Fe_{0.6}O_3$	13.4
$LaCo_{0.8}Mn_{0.2}O_3$	31	$La_{0.8}Ce_{0.2}Ni_{0.4}Fe_{0.6}O_3$	21.7
$La_{0.9}Zn_{0.1}MnO_3$	28.3	$LaMn_{0.3}Cu_{0.7}O_3$	34

化学式	SSA/ m^2g^{-1}	化学式	SSA/ m^2g^{-1}
$La_{0.8}Zn_{0.2}MnO_3$	26.4	$LaMn_{0.3}Fe_{0.7}O_3$	31
$La_{0.7}Zn_{0.3}MnO_3$	20.6	$La_{0.8}Sr_{0.2}Mn_{0.3}Cu_{0.7}O_3$	26
$La_{0.6}Zn_{0.4}MnO_3$	13	$La_{0.8}Ce_{0.2}Mn_{0.3}Cu_{0.7}O_3$	25
$La_{0.5}Zn_{0.5}MnO_3$	9.2	$La_{0.8}Sr_{0.2}Mn_{0.3}Fe_{0.7}O_3$	24
$La_{0.4}Zn_{0.6}MnO_3$	7.7	$La_{0.8}Ce_{0.2}Mn_{0.3}Fe_{0.7}O_3$	27
$La_{0.78}K_{0.02}Sr_{0.2}MnO_3$	8.4	$LaMn_{0.9}Cu_{0.1}O_3$	36
$La_{0.74}K_{0.06}Sr_{0.2}MnO_3$	5.3	$LaMn_{0.5}Cu_{0.5}O_3$	34
$La_{0.7}K_{0.1}Sr_{0.2}MnO_3$	5.7	$LaMn_{0.9}Fe_{0.1}O_3$	33
$La_{0.66}K_{0.14}Sr_{0.2}MnO_3$	6.3	$LaMn_{0.5}Fe_{0.5}O_3$	27
$La_{0.62}K_{0.18}Sr_{0.2}MnO_3$	10.2	$La_{0.4}Sr_{0.6}MnO_3$	83.7
$La_{0.6}K_{0.2}Sr_{0.2}MnO_3$	8.7	$La_{0.2}Sr_{0.8}MnO_3$	114.3
$LaNi_{0.95}Ti_{0.05}O_3$	4.527	$Al_{0.05}La_{0.95}MnO_3$	27.7
$LaNi_{0.9}Ti_{0.1}O_3$	2.516	$Al_{0.1}La_{0.9}MnO_3$	39.7
$LaNi_{0.85}Ti_{0.15}O_3$	3.891	$Al_{0.15}La_{0.85}MnO_3$	42.5
$LaNi_{0.8}Ti_{0.2}O_3$	4.584	$Al_{0.2}La_{0.8}MnO_3$	47.3
$LaCu_{0.2}Fe_{0.8}O_3$	7.85	$Al_{0.3}La_{0.7}MnO_3$	38.5
$LaAl_{0.2}Fe_{0.8}O_3$	6.42	$LaCu_{0.7}Zn_{0.3}O_3$	0.7
$LaCo_{0.75}Mn_{0.25}O_3$	8	$La_{0.8}Y_{0.2}Cu_{0.7}Zn_{0.3}O_3$	1.3
$LaCo_{0.75}Ni_{0.25}O_3$	10	$La_{0.8}Mg_{0.2}Cu_{0.7}Zn_{0.3}O_3$	1.2
$LaCo_{0.5}Ni_{0.5}O_3$	8	$La_{0.8}Ce_{0.2}Cu_{0.7}Zn_{0.3}O_3$	2.3
$LaCo_{0.25}Ni_{0.75}O_3$	12	$La_{0.8}Zr_{0.2}Cu_{0.7}Zn_{0.3}O_3$	0.7
$LaNi_{0.25}Fe_{0.75}O_3$	7	$La_{0.6}Pb_{0.2}Mg_{0.2}MnO_3$	8.6
$LaNi_{0.5}Fe_{0.5}O_3$	6	$LaFe_{0.75}Mn_{0.25}O_3$	25.9
$LaNi_{0.75}Fe_{0.25}O_3$	7	$LaFe_{0.5}Mn_{0.5}O_3$	25.2
$LaCrO_3$	8.1	$LaFe_{0.25}Mn_{0.75}O_3$	28.2
$La_{0.8}Ce_{0.2}Mn_{0.9}Co_{0.1}O_3$	13.8	$La_{0.9}Sr_{0.1}MnO_3$	31.2
$La_{0.8}Ce_{0.2}Mn_{0.7}Co_{0.3}O_3$	4.503	$La_{0.9}Sm_{0.1}NiO_3$	5.4
$La_{0.8}Ce_{0.2}Mn_{0.5}Co_{0.5}O_3$	9.219	$La_{0.5}Sm_{0.5}NiO_3$	3.4
$La_{0.8}Ce_{0.2}Mn_{0.3}Co_{0.7}O_3$	5.712	$La_{0.1}Sm_{0.9}NiO_3$	8.4
$La_{0.8}Ca_{0.2}MnO_3$	20.5	$Pb_{0.8}Ba_{0.2}TiO_3$	6.228
$La_{0.67}Ca_{0.33}MnO_3$	10.7	$Pb_{0.6}Ba_{0.4}TiO_3$	6.514
$La_{0.5}Ca_{0.5}MnO_3$	23	$Pb_{0.5}Ba_{0.5}TiO_3$	10.484
$La_{0.25}Ca_{0.75}MnO_3$	20.8	$Pb_{0.4}Ba_{0.6}TiO_3$	13.708
$CaMnO_3$	7.1	$Pb_{0.2}Ba_{0.8}TiO_3$	16.592

化学式	SSA/ m^2g^{-1}	化学式	SSA/ m^2g^{-1}
$La_{0.9}Ce_{0.1}Ni_{0.9}Zr_{0.1}O_3$	3	$La_{0.8}Ce_{0.2}Mn_{0.6}Cu_{0.4}O_3$	12.3
$La_{0.9}Ce_{0.1}Ni_{0.8}Zr_{0.2}O_3$	5	$La_{0.8}Ce_{0.2}Mn_{0.7}Cu_{0.3}O_3$	22.2
$PrMn_{0.8}Fe_{0.2}O_3$	8.34	$La_{0.8}Ce_{0.2}Mn_{0.8}Cu_{0.2}O_3$	12.8
$PrMn_{0.6}Fe_{0.4}O_3$	11.67	$La_{0.8}Sr_{0.2}Mn_{0.6}Cu_{0.4}O_3$	28
$PrMn_{0.4}Fe_{0.6}O_3$	14.25	$La_{0.8}Ce_{0.1}Sr_{0.1}Mn_{0.6}Cu_{0.4}O_3$	12.4
$PrMn_{0.2}Fe_{0.8}O_3$	8.05		

表 S9 E_g 回归模型训练数据集

Table S9 Training data of the E_g regression model

化学式	E_g/eV	化学式	E_g/eV
$PrCuO_3$	3.256	$Bi_{0.9}Gd_{0.1}Fe_{0.9}Cr_{0.1}O_3$	2.6
$PrCu_{0.9}Zn_{0.1}O_3$	3.088	$Pb_{0.8}Co_{0.15}La_{0.05}TiO_3$	3.02
$PrCu_{0.8}Zn_{0.2}O_3$	2.933	$Pb_{0.8}Co_{0.1}La_{0.1}TiO_3$	3.01
$PrCu_{0.7}Zn_{0.3}O_3$	2.898	$Pb_{0.8}Co_{0.05}La_{0.15}TiO_3$	2.32
$DyCr_{0.9}Co_{0.1}O_3$	2.86	$Pb_{0.8}La_{0.2}TiO_3$	3.2
$DyCr_{0.8}Co_{0.2}O_3$	2.2	$Bi_{0.99}Ba_{0.01}FeO_3$	2.38
$DyCr_{0.7}Co_{0.3}O_3$	2.17	$Bi_{0.98}Ba_{0.02}FeO_3$	2.36
$LaFe_{0.75}Cr_{0.25}O_3$	1.86	$Bi_{0.97}Ba_{0.03}FeO_3$	2.21
$LaFe_{0.5}Cr_{0.5}O_3$	1.82	$Bi_{0.96}Ba_{0.04}FeO_3$	2.04
$LaFe_{0.25}Cr_{0.75}O_3$	1.92	$Bi_{0.95}Ba_{0.05}FeO_3$	1.97
$Bi_{0.85}Gd_{0.15}FeO_3$	1.6	$La_{0.95}Na_{0.05}FeO_3$	3.07
$La_{0.95}Ba_{0.05}FeO_3$	2.29	$La_{0.9}Na_{0.1}FeO_3$	2.81
$La_{0.9}Ba_{0.1}FeO_3$	2.4	$La_{0.85}Na_{0.15}FeO_3$	2.97
$La_{0.8}Ba_{0.2}FeO_3$	2.16	$BaZr_{0.05}Ti_{0.95}O_3$	3.36
$La_{0.95}Ca_{0.05}FeO_3$	2.34	$BaZr_{0.1}Ti_{0.9}O_3$	3.68
$La_{0.9}Ca_{0.1}FeO_3$	2.35	$BaZr_{0.15}Ti_{0.85}O_3$	3.71
$La_{0.8}Ca_{0.2}FeO_3$	2.36	$BaZr_{0.2}Ti_{0.8}O_3$	3.57
$La_{0.7}Ca_{0.3}FeO_3$	2.27	$Bi_{0.9}Ho_{0.1}Fe_{0.95}Mn_{0.05}O_3$	1.79
$La_{0.6}Ca_{0.4}FeO_3$	2.26	$Bi_{0.9}Ho_{0.1}Fe_{0.95}Co_{0.05}O_3$	1.7
$La_{0.95}Sr_{0.05}FeO_3$	2.25	$Bi_{0.9}Ho_{0.1}Fe_{0.95}Cu_{0.05}O_3$	2.03
$La_{0.9}Sr_{0.1}FeO_3$	2.35	$Bi_{0.9}Ho_{0.1}Fe_{0.95}Zn_{0.05}O_3$	1.96
$La_{0.8}Sr_{0.2}FeO_3$	2.19	$Bi_{0.9}Ho_{0.1}Fe_{0.95}Ni_{0.05}O_3$	1.89
$La_{0.95}Mg_{0.05}FeO_3$	2.17	$Bi_{0.9}Ho_{0.1}Fe_{0.95}Cr_{0.05}O_3$	1.94
$La_{0.9}Mg_{0.1}FeO_3$	2.25	$LaMn_{0.2}Fe_{0.8}O_3$	2.49
$La_{0.8}Mg_{0.2}FeO_3$	2.29	$LaMn_{0.2}Cr_{0.2}Fe_{0.6}O_3$	2.51
$La_{0.7}Mg_{0.3}FeO_3$	2.51	$LaMn_{0.2}Co_{0.2}Fe_{0.6}O_3$	2.32
$La_{0.6}Mg_{0.4}FeO_3$	2.34	$LaMn_{0.2}Ni_{0.2}Fe_{0.6}O_3$	2.3
$Bi_{0.75}La_{0.25}FeO_3$	1.85	$LaMn_{0.2}Cu_{0.2}Fe_{0.6}O_3$	2.29
$LaFe_{0.6}Co_{0.4}O_3$	2.39	$LaMn_{0.2}Zn_{0.2}Fe_{0.6}O_3$	2.19
$LaFe_{0.5}Co_{0.5}O_3$	2.31	$LaMnO_3$	2.67

化学式	E_g/eV	化学式	E_g/eV
$LaFe_{0.4}Co_{0.6}O_3$	2.37	$Gd_{0.9}Dy_{0.1}CrO_3$	3.11
$Ba_{0.99}Li_{0.005}La_{0.005}TiO_3$	3.02	$Gd_{0.5}Dy_{0.5}CrO_3$	3.06
$Ba_{0.98}Li_{0.01}La_{0.01}TiO_3$	2.95	$Gd_{0.3}Dy_{0.7}CrO_3$	3.03
$Ba_{0.97}Li_{0.015}La_{0.015}TiO_3$	2.84	$Gd_{0.1}Dy_{0.9}CrO_3$	2.99
$Ba_{0.96}Li_{0.02}La_{0.02}TiO_3$	2.77	$BiMnO_3$	1.31
$PrCrO_3$	3.24	$BiMn_{0.9}Cr_{0.1}O_3$	1.32
$LaGd_{0.02}Fe_{0.98}O_3$	2.6	$BiMn_{0.9}Fe_{0.1}O_3$	1.33
$LaGd_{0.04}Fe_{0.96}O_3$	2.58	$BiMn_{0.9}Co_{0.1}O_3$	1.36
$LaGd_{0.06}Fe_{0.94}O_3$	2.53	$BiMn_{0.9}Zn_{0.1}O_3$	1.37
$LaGd_{0.08}Fe_{0.92}O_3$	2.52	$HoCrO_3$	3.45
$LaGd_{0.1}Fe_{0.9}O_3$	2.46	$HoCr_{0.7}Fe_{0.3}O_3$	3.39
$LaDy_{0.02}Fe_{0.98}O_3$	2.59	$BaZrO_3$	3.6553
$LaDy_{0.04}Fe_{0.96}O_3$	2.58	$BaZr_{0.95}Fe_{0.05}O_3$	3.4943
$LaDy_{0.06}Fe_{0.94}O_3$	2.57	$BaZr_{0.9}Fe_{0.1}O_3$	3.4277
$LaDy_{0.08}Fe_{0.92}O_3$	2.52	$BaZr_{0.8}Fe_{0.2}O_3$	3.3207
$LaDy_{0.1}Fe_{0.9}O_3$	2.5	$BaZr_{0.7}Fe_{0.3}O_3$	3.2201
$LaNd_{0.02}Fe_{0.98}O_3$	2.6	$BaZr_{0.6}Fe_{0.4}O_3$	3.0032
$LaNd_{0.04}Fe_{0.96}O_3$	2.59	$BaZr_{0.5}Fe_{0.5}O_3$	2.8435
$LaNd_{0.06}Fe_{0.94}O_3$	2.54	$BaSnO_3$	3.09
$LaNd_{0.08}Fe_{0.92}O_3$	2.52	$LaCo_{0.2}Fe_{0.8}O_3$	1.78
$LaNd_{0.1}Fe_{0.9}O_3$	2.52	$LaCo_{0.4}Fe_{0.6}O_3$	1.7
$Bi_{0.95}Ca_{0.05}FeO_3$	2.2	$LaCo_{0.6}Fe_{0.4}O_3$	1.68
$Bi_{0.95}Ca_{0.05}Fe_{0.95}Ni_{0.05}O_3$	2.17	$LaCo_{0.8}Fe_{0.2}O_3$	1.8
$Bi_{0.98}Ce_{0.02}FeO_3$	2.01	$Bi_{0.05}Ca_{0.95}FeO_3$	2.19
$Bi_{0.96}Ce_{0.04}FeO_3$	2	$Bi_{0.1}Ca_{0.9}FeO_3$	2.23
$Bi_{0.94}Ce_{0.06}FeO_3$	1.97	$Bi_{0.15}Ca_{0.85}FeO_3$	2.35
$La_{0.95}Ce_{0.05}FeO_3$	2.8	$Bi_{0.2}Ca_{0.8}FeO_3$	2.36
$La_{0.9}Ce_{0.1}FeO_3$	2.54	$Bi_{0.95}Ca_{0.05}Fe_{0.95}Ti_{0.05}O_3$	1.82
$La_{0.85}Ce_{0.15}FeO_3$	1.89	$Bi_{0.9}Ca_{0.1}Fe_{0.9}Ti_{0.1}O_3$	1.96
$GdMn_{0.7}Ni_{0.3}O_3$	3.2	$Bi_{0.85}Ca_{0.15}Fe_{0.85}Ti_{0.15}O_3$	2.08
$GdCr_{0.9}Mn_{0.1}O_3$	3.77	$Bi_{0.8}Ca_{0.2}Fe_{0.8}Ti_{0.2}O_3$	2.14
$GdCr_{0.8}Mn_{0.2}O_3$	3.72	$Bi_{0.75}Ca_{0.25}Fe_{0.75}Ti_{0.25}O_3$	2.25
$GdCr_{0.7}Mn_{0.3}O_3$	3.69	$Bi_{0.9}Y_{0.1}FeO_3$	2.5
$GdCr_{0.6}Mn_{0.4}O_3$	3.71	$Bi_{0.9}Y_{0.1}Fe_{0.97}Co_{0.03}O_3$	2.42
$Bi_{0.98}Ho_{0.02}Fe_{0.99}Cr_{0.01}O_3$	2.22	$Bi_{0.9}Y_{0.1}Fe_{0.95}Co_{0.05}O_3$	2.42
$Bi_{0.98}Ho_{0.02}Fe_{0.98}Cr_{0.02}O_3$	2.66	$Bi_{0.9}Y_{0.1}Fe_{0.9}Co_{0.1}O_3$	2.45
$Bi_{0.98}Ho_{0.02}Fe_{0.97}Cr_{0.03}O_3$	2.37	$BiFe_{0.95}Co_{0.05}O_3$	1.95
$Bi_{0.98}Ho_{0.02}Fe_{0.96}Cr_{0.04}O_3$	2.7	$BiFe_{0.85}Co_{0.15}O_3$	1.91
$Bi_{0.98}La_{0.02}FeO_3$	1.99	$BiFe_{0.8}Co_{0.2}O_3$	1.64
$Bi_{0.98}La_{0.02}Fe_{0.9}Se_{0.1}O_3$	1.96	$BiFe_{0.75}Co_{0.25}O_3$	1.28
$Bi_{0.98}La_{0.02}Fe_{0.75}Se_{0.25}O_3$	1.8	$Bi_{0.95}Ho_{0.05}FeO_3$	2.09
$Bi_{0.98}La_{0.02}Fe_{0.5}Se_{0.5}O_3$	1.77	$Bi_{0.85}Ho_{0.15}FeO_3$	2.03
$Bi_{0.98}La_{0.02}SeO_3$	2.05	$Bi_{0.8}Ho_{0.2}FeO_3$	2.01

化学式	E_g/eV	化学式	E_g/eV
$LaNi_{0.2}Fe_{0.8}O_3$	1.63	$Bi_{0.9}Nd_{0.1}FeO_3$	2.89
$LaNi_{0.4}Fe_{0.6}O_3$	1.56	$Bi_{0.9}Nd_{0.1}Fe_{0.9}Co_{0.1}O_3$	2.93
$LaNi_{0.6}Fe_{0.4}O_3$	1.65	$BiFe_{0.95}Mn_{0.05}O_3$	2.6
$LaNi_{0.8}Fe_{0.2}O_3$	1.77	$Bi_{0.97}Sm_{0.03}Fe_{0.95}Mn_{0.05}O_3$	2.62
$NdFeO_3$	3.35	$Bi_{0.94}Sm_{0.06}Fe_{0.95}Mn_{0.05}O_3$	2.65
$NdFe_{0.9}Co_{0.1}O_3$	3.26	$Bi_{0.91}Sm_{0.09}Fe_{0.95}Mn_{0.05}O_3$	2.67
$NdFe_{0.8}Co_{0.2}O_3$	3.2	$Bi_{0.9}Gd_{0.1}Fe_{0.95}Mn_{0.05}O_3$	1.76
$NdFe_{0.7}Co_{0.3}O_3$	3.09	$Bi_{0.9}Gd_{0.1}Fe_{0.9}Mn_{0.1}O_3$	1.62
$NdFe_{0.6}Co_{0.4}O_3$	3.04	$Bi_{0.9}Gd_{0.1}Fe_{0.85}Mn_{0.15}O_3$	1.68
$La_{0.75}Ba_{0.25}FeO_3$	2.98	$Bi_{0.9}Gd_{0.1}Fe_{0.8}Mn_{0.2}O_3$	1.52
$La_{0.75}Ba_{0.2}Sr_{0.05}FeO_3$	3.09	$Bi_{0.9}Gd_{0.1}Fe_{0.75}Mn_{0.25}O_3$	1.47
$La_{0.75}Ba_{0.15}Sr_{0.1}FeO_3$	3.2	$Bi_{0.9}Ca_{0.1}FeO_3$	2.47
$La_{0.75}Ba_{0.1}Sr_{0.15}FeO_3$	3.25	$Bi_{0.8}Ca_{0.2}FeO_3$	2.43
$BaTi_{0.75}Mn_{0.25}O_3$	2.93	$Bi_{0.7}Ca_{0.3}FeO_3$	2.385
$BaTi_{0.5}Mn_{0.5}O_3$	2.83	$Bi_{0.6}Ca_{0.4}FeO_3$	2.38
$BaTi_{0.25}Mn_{0.75}O_3$	2.71	$Bi_{0.5}Ca_{0.5}FeO_3$	2.37
$YbFeO_3$	1.55	$La_{0.9}Sr_{0.1}Fe_{0.9}Ni_{0.1}O_3$	2.28
$Bi_{0.9}Gd_{0.1}Fe_{0.975}Cr_{0.025}O_3$	2.56	$La_{0.8}Sr_{0.2}Fe_{0.8}Ni_{0.2}O_3$	2.36
$Bi_{0.9}Gd_{0.1}Fe_{0.95}Cr_{0.05}O_3$	2.58	$Bi_{0.85}Nd_{0.15}FeO_3$	2.8
$Bi_{0.9}Gd_{0.1}Fe_{0.925}Cr_{0.075}O_3$	2.59		

表 S10 T_c 回归模型训练数据集

Table S10 Training data of the T_c regression model

化学式	T_c/K	化学式	T_c/K
$La_{0.67}Sr_{0.33}MnO_3$	355	$Pb_{0.86}Gd_{0.08}La_{0.06}Zr_{0.52}Ti_{0.48}O_3$	347
$La_{0.67}Sr_{0.23}K_{0.1}MnO_3$	360	$La_{0.603}Pr_{0.067}Pb_{0.33}MnO_3$	353
$La_{0.67}Sr_{0.23}Pb_{0.1}MnO_3$	365	$La_{0.536}Pr_{0.134}Pb_{0.33}MnO_3$	346
$La_{0.7}Ba_{0.15}Sr_{0.15}CoO_3$	228	$La_{0.469}Pr_{0.201}Pb_{0.33}MnO_3$	330
$Ba_{0.8}Sr_{0.2}TiO_3$	351.15	$La_{0.765}Sm_{0.085}K_{0.15}MnO_3$	170
$Ba_{0.7}Sr_{0.3}TiO_3$	306.65	$La_{0.68}Sm_{0.17}K_{0.15}MnO_3$	145
$Ba_{0.6}Sr_{0.4}TiO_3$	269.65	$La_{0.595}Sm_{0.255}K_{0.15}MnO_3$	130
$Ba_{0.5}Sr_{0.5}TiO_3$	231.48	$La_{0.7}Ca_{0.15}Ba_{0.15}MnO_3$	299.2
$Ba_{0.4}Sr_{0.6}TiO_3$	189.15	$La_{0.67}Ca_{0.33}MnO_3$	272
$La_{0.8}Ba_{0.05}Sr_{0.15}MnO_3$	320	$La_{0.67}Dy_{0.03}Sr_{0.3}MnO_3$	274.94
$La_{0.75}K_{0.05}Ba_{0.05}Sr_{0.15}MnO_3$	335	$La_{0.7}Nd_{0.05}Ba_{0.25}MnO_3$	293
$La_{0.7}K_{0.1}Ba_{0.05}Sr_{0.15}MnO_3$	345	$La_{0.7}Nd_{0.1}Ba_{0.2}MnO_3$	257
$La_{0.65}K_{0.15}Ba_{0.05}Sr_{0.15}MnO_3$	355	$La_{0.6}Gd_{0.1}Sr_{0.3}MnO_3$	350
$La_{0.6}K_{0.2}Ba_{0.05}Sr_{0.15}MnO_3$	360	$La_{0.65}Ca_{0.2}Na_{0.075}K_{0.075}MnO_3$	296
$La_{0.6}Nd_{0.1}Ca_{0.3}MnO_3$	171	$La_{0.67}Sr_{0.22}Ba_{0.11}MnO_3$	360
$La_{0.6}Sm_{0.1}Ca_{0.3}MnO_3$	135	$La_{0.67}Sr_{0.22}Ba_{0.11}Mn_{0.9}Co_{0.1}O_3$	300

化学式	T_c/K	化学式	T_c/K
$La_{0.6}Gd_{0.1}Ca_{0.3}MnO_3$	125	$La_{0.67}Sr_{0.22}Ba_{0.11}Mn_{0.8}Co_{0.2}O_3$	220
$La_{0.6}Dy_{0.1}Ca_{0.3}MnO_3$	111	$La_{0.67}Sr_{0.22}Ba_{0.11}Mn_{0.7}Co_{0.3}O_3$	185
$La_{0.6}Ca_{0.2}Na_{0.2}MnO_3$	275	$La_{0.765}Pr_{0.085}K_{0.15}MnO_3$	225
$La_{0.7}Sr_{0.3}Mn_{0.9}Cu_{0.1}O_3$	320	$La_{0.595}Pr_{0.255}K_{0.15}MnO_3$	183
$La_{0.6}Bi_{0.1}Sr_{0.3}Mn_{0.9}Cu_{0.1}O_3$	300	$La_{0.425}Pr_{0.425}K_{0.15}MnO_3$	158
$La_{0.6}Bi_{0.1}Sr_{0.25}Ca_{0.05}Mn_{0.9}Cu_{0.1}O_3$	290	$Pr_{0.8}Na_{0.15}K_{0.05}MnO_3$	180
$La_{0.67}Ca_{0.33}Mn_{0.98}Ni_{0.02}O_3$	244	$Pr_{0.8}Na_{0.1}K_{0.1}MnO_3$	175
$La_{0.8}Na_{0.2}MnO_3$	297	$Pr_{0.8}Na_{0.05}K_{0.15}MnO_3$	160
$La_{0.8}Na_{0.2}Mn_{0.97}Ni_{0.03}O_3$	275	$La_{0.7}Ca_{0.21}Ag_{0.09}MnO_3$	263
$La_{0.8}Na_{0.2}Mn_{0.94}Ni_{0.06}O_3$	257	$La_{0.7}Ca_{0.15}Sr_{0.15}Mn_{0.875}Ga_{0.125}O_3$	221.4
$La_{0.9}Sr_{0.1}MnO_3$	154.8	$La_{0.7}Ca_{0.15}Sr_{0.15}Mn_{0.85}Ga_{0.15}O_3$	208.21
$La_{0.85}Sr_{0.15}MnO_3$	235.8	$La_{0.7}Ca_{0.15}Sr_{0.15}Mn_{0.825}Ga_{0.175}O_3$	166.18
$La_{0.8}Sr_{0.2}MnO_3$	305.9	$La_{0.7}Ca_{0.15}Sr_{0.15}Mn_{0.8}Ga_{0.2}O_3$	137.7
$La_{0.8}Ag_{0.2}MnO_3$	306	$La_{0.65}Sr_{0.35}MnO_3$	362
$La_{0.7}Ca_{0.29}K_{0.01}MnO_3$	265.01	$La_{0.603}Sm_{0.067}Pb_{0.33}MnO_3$	341
$La_{0.7}Ca_{0.28}K_{0.02}MnO_3$	266.02	$La_{0.536}Sm_{0.134}Pb_{0.33}MnO_3$	311
$La_{0.7}Ca_{0.27}K_{0.03}MnO_3$	270.01	$La_{0.469}Sm_{0.201}Pb_{0.33}MnO_3$	286
$La_{0.7}Ca_{0.26}K_{0.04}MnO_3$	277.01	$NdMnO_3$	67.2
$La_{0.67}Ca_{0.29}Sr_{0.04}MnO_3$	276	$Nd_{0.85}Na_{0.15}MnO_3$	99.1
$La_{0.8}Na_{0.2}Mn_{0.97}Bi_{0.03}O_3$	257	$Nd_{0.85}K_{0.15}MnO_3$	98.6
$La_{0.65}Ca_{0.35}Mn_{0.95}Ni_{0.05}O_3$	272	$Pr_{0.6}La_{0.1}Mg_{0.3}MnO_3$	64
$La_{0.65}Ca_{0.35}Mn_{0.9}Ni_{0.1}O_3$	236	$Pr_{0.6}La_{0.1}Mg_{0.3}Mn_{0.9}Fe_{0.1}O_3$	65
$La_{0.65}Ca_{0.35}Mn_{0.85}Ni_{0.15}O_3$	194	$Pr_{0.6}La_{0.1}Mg_{0.3}Mn_{0.7}Fe_{0.3}O_3$	380
$Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3$	385.15	$La_{0.7}Sr_{0.21}K_{0.09}MnO_3$	295
$BaTiO_3$	403.46	$Pr_{0.6}La_{0.1}Ca_{0.3}MnO_3$	94
$Ba_{0.96}Ca_{0.04}TiO_3$	413.28	$Pr_{0.6}La_{0.1}Ca_{0.3}Mn_{0.9}Fe_{0.1}O_3$	65
$Ba_{0.95}Ca_{0.05}TiO_3$	416.91	$Pr_{0.6}La_{0.1}Ca_{0.3}Mn_{0.8}Fe_{0.2}O_3$	60
$Ba_{0.9}Ca_{0.1}TiO_3$	414.53	$Pr_{0.6}La_{0.1}Ca_{0.3}Mn_{0.7}Fe_{0.3}O_3$	59
$La_{0.595}Gd_{0.005}Sr_{0.4}MnO_3$	354.7	$La_{0.7}Sr_{0.3}Mn_{0.9}Fe_{0.1}O_3$	261
$La_{0.5}Gd_{0.1}Sr_{0.4}MnO_3$	336.3	$La_{0.7}Pb_{0.3}Mn_{0.9}Fe_{0.1}O_3$	215
$La_{0.5}Ba_{0.5}MnO_3$	339	$La_{0.7}Ba_{0.3}Mn_{0.9}Fe_{0.1}O_3$	194
$La_{0.603}Pr_{0.067}Ca_{0.33}MnO_3$	233	$Pr_{0.67}Ca_{0.33}FeO_3$	208
$La_{0.536}Pr_{0.134}Ca_{0.33}MnO_3$	228	$Pr_{0.67}Ca_{0.33}Fe_{0.1}Mn_{0.9}O_3$	176
$La_{0.469}Pr_{0.201}Ca_{0.33}MnO_3$	180	$Pr_{0.67}Ca_{0.33}Fe_{0.2}Mn_{0.8}O_3$	135
$La_{0.402}Pr_{0.268}Ca_{0.33}MnO_3$	171	$Pr_{0.67}Ca_{0.33}Fe_{0.3}Mn_{0.7}O_3$	105
$Pb_{0.94}La_{0.06}Zr_{0.52}Ti_{0.48}O_3$	350	$La_{0.65}Ca_{0.35}MnO_3$	267.9
$Pb_{0.92}Gd_{0.02}La_{0.06}Zr_{0.52}Ti_{0.48}O_3$	373	$La_{0.67}Pb_{0.28}Ag_{0.05}MnO_3$	332
$Pb_{0.9}Gd_{0.04}La_{0.06}Zr_{0.52}Ti_{0.48}O_3$	366	$La_{0.67}Pb_{0.23}Ag_{0.1}MnO_3$	311
$Pb_{0.88}Gd_{0.06}La_{0.06}Zr_{0.52}Ti_{0.48}O_3$	399	$La_{0.67}Pb_{0.18}Ag_{0.15}MnO_3$	290

表 S11 *tanδ* 回归模型训练数据集

Table S11 Training data of the *tanδ* regression model

化学式	*tanδ*	化学式	*tanδ*
$MnFeO_3$	0.13	$Na_{0.47}Bi_{0.47}Ba_{0.06}TiO_3$	0.048
$Gd_{0.4}Mn_{0.6}Fe_{0.96}Cu_{0.04}O_3$	0.12	$Pb_{0.94}La_{0.06}Zr_{0.52}Ti_{0.48}O_3$	0.03
$Gd_{0.6}Mn_{0.4}Fe_{0.94}Cu_{0.06}O_3$	0.1	$Pb_{0.92}Gd_{0.02}La_{0.06}Zr_{0.52}Ti_{0.48}O_3$	0.027
$Gd_{0.8}Mn_{0.2}Fe_{0.92}Cu_{0.08}O_3$	0.08	$Pb_{0.90}Gd_{0.04}La_{0.06}Zr_{0.52}Ti_{0.48}O_3$	0.032
$Na_{0.425}K_{0.075}Bi_{0.5}TiO_3$	0.051	$Pb_{0.88}Gd_{0.06}La_{0.06}Zr_{0.52}Ti_{0.48}O_3$	0.029
$Pb_{0.5}Sr_{0.5}TiO_3$	0.056	$Pb_{0.86}Gd_{0.08}La_{0.06}Zr_{0.52}Ti_{0.48}O_3$	0.028
$Pb_{0.5}Sr_{0.5}Ti_{0.99}Fe_{0.01}O_3$	0.045	$Ba_{0.95}Tm_{0.05}TiO_3$	0.0231
$Pb_{0.5}Sr_{0.5}Ti_{0.95}Fe_{0.05}O_3$	0.044	$Bi_{0.9}Sm_{0.1}FeO_3$	0.08
$Pb_{0.5}Sr_{0.5}Ti_{0.9}Fe_{0.1}O_3$	0.016	$BiFeO_3$	0.065
$Ba_{0.95}La_{0.05}TiO_3$	0.005	$BiFe_{0.97}Ti_{0.03}O_3$	0.061
$Pb_{0.9}Na_{0.05}Sm_{0.05}TiO_3$	0.012	$Na_{0.5}K_{0.5}NbO_3$	0.05
$Pb_{0.8}Na_{0.1}Sm_{0.1}TiO_3$	0.017	$Ba_{0.7}Sr_{0.3}Zr_{0.01}Ti_{0.99}O_3$	0.06
$Pb_{0.7}Na_{0.15}Sm_{0.15}TiO_3$	0.026	$Ba_{0.7}Sr_{0.3}Zr_{0.02}Ti_{0.98}O_3$	0.05
$Pb_{0.6}Na_{0.2}Sm_{0.2}TiO_3$	0.038	$Ba_{0.7}Sr_{0.3}Zr_{0.03}Ti_{0.97}O_3$	0.02
$Pb_{0.5}Na_{0.25}Sm_{0.25}TiO_3$	0.037		

表 S12 *SSA* 模型测试集模型预报值与实验值

Table S12: Predicted and experimental *SSA* with the lowest error of the testing set

化学式	Pred. *SSA*/ m^2g^{-1}	Exp. *SSA*/ m^2g^{-1}
$LaMnO_3$	31.854	30.8
$LaCo_{0.5}Mn_{0.5}O_3$	19.938	7
$LaCoO_3$	5.401	5
$La_{0.8}Sr_{0.2}MnO_3$	19.049	8.3
$LaTi_{0.2}Fe_{0.8}O_3$	27.675	12.95
$LaNiO_3$	7.506	8
$LaFeO_3$	14.869	10
$LaMn_{0.7}Cu_{0.3}O_3$	30.441	29
$LaMn_{0.7}Fe_{0.3}O_3$	31.199	31
$La_{0.8}Ce_{0.2}MnO_3$	18.215	10.727

表 S13 E_g 模型测试集模型预报值与实验值

Table S13: Predicted and experimental E_g with the lowest error of the testing set

化学式	Pred. E_g/eV	Exp. E_g/eV
$BiFeO_3$	2.188	2.18
$BiFe_{0.9}Co_{0.1}O_3$	2.163	1.81

化学式	Pred. E_g/eV	Exp. E_g/eV
$DyCrO_3$	2.902	2.96
$LaFeO_3$	2.373	2.52
$LaCrO_3$	2.433	2.34
$GdCrO_3$	3.443	3.36
$LaNiO_3$	1.572	1.8
$BaTiO_3$	3.019	3.13
$Bi_{0.9}Gd_{0.1}FeO_3$	2.101	2.07

表 S14 T_c 模型测试集模型预报值与实验值

Table S14: Predicted and experimental T_c with the lowest error of the testing set

化学式	Pred. T_c/K	Exp. T_c/K
$La_{0.7}Ca_{0.3}MnO_3$	237.942	215
$La_{0.67}Pb_{0.33}MnO_3$	340.995	349
$La_{0.75}Sr_{0.25}MnO_3$	323.147	344.9
$La_{0.6}Sr_{0.4}MnO_3$	371.224	366.53
$La_{0.85}K_{0.15}MnO_3$	227.954	238
$La_{0.7}Sr_{0.3}MnO_3$	347.070	361.5
$La_{0.7}Ba_{0.3}MnO_3$	311.931	303
$La_{0.7}Ca_{0.15}Sr_{0.15}MnO_3$	296.484	319.2

表 S15 $tan\delta$ 模型测试集模型预报值与实验值

Table S15: Predicted and experimental $tan\delta$ with the lowest error of the testing set

化学式	Pred. $tan\delta$	Exp. $tan\delta$
$Bi_{0.5}Na_{0.5}TiO_3$	0.052	0.07
$BaTiO_3$	0.032	0.1

表 S16 *SSA* 模型可疑样本模型预报值与实验值

Table S16: Predicted and experimental *SSA* of the suspected samples

化学式	Pred. *SSA*/ m^2g^{-1}	Exp. *SSA*/ m^2g^{-1}
$CaFeO_3$	13.951	17.37
$Ca_{0.5}Pr_{0.5}FeO_3$	24.595	66.65
$La_{0.6}Sr_{0.4}MnO_3$	33.944	96.4

表 S17 E_g 模型可疑样本模型预报值与实验值

Table S17: Predicted and experimental E_g of the suspected samples

化学式	Pred. E_g/eV	Exp. E_g/eV
$LaNi_{0.8}Co_{0.2}O_3$	1.598	3.825
$LaNi_{0.6}Co_{0.4}O_3$	1.642	3.826
$LaNi_{0.4}Co_{0.6}O_3$	1.703	3.82
$CoFeO_3$	3.268	1.84

表 S18 T_c 模型可疑样本模型预报值与实验值

Table S18: Predicted and experimental T_c of the suspected samples

化学式	Pred. T_c/K	Exp. T_c/K
$Pr_{0.6}La_{0.1}Mg_{0.3}Mn_{0.8}Fe_{0.2}O_3$	266.598	957

表 S19 $tan\delta$ 模型可疑样本模型预报值与实验值

Table S19: Predicted and experimental $tan\delta$ of the suspected samples

化学式	Pred. $tan\delta$	Exp. $tan\delta$
$Gd_{0.2}Mn_{0.8}Fe_{0.98}Cu_{0.02}O_3$	0.119	0.2
$GdFe_{0.9}Cu_{0.1}O_3$	0.077	0.129
$Na_{0.5}Ba_{0.5}Ti_{0.99}W_{0.01}O_3$	0.053	0.094
$SrTiO_3$	0.053	0.45
$Bi_{0.5}K_{0.5}TiO_3$	0.035	0.0584
$BaTi_{0.98}Ni_{0.02}O_3$	0.032	0.27
$BaTi_{0.96}Ni_{0.04}O_3$	0.033	0.16
$BaTi_{0.94}Ni_{0.06}O_3$	0.034	0.11
$Ba_{0.7}Sr_{0.3}TiO_3$	0.039	0.27

表 S20 ABO_3 型钙钛矿氧离子电导率样本化学式及其氧离子电导率

Table S20: The chemical formula of the ABO_3 type perovskites and corresponding oxide ionic conductivity of the data set collected form publications

化学式	$ln\sigma$	化学式	$ln\sigma$
$BaZrO_{3-\delta}$	-14	$La_{0.5}Sr_{0.5}Ga_{0.65}Zr_{0.35}O_{3-\delta}$	-4.93
$PrGaO_{3-\delta}$	-12.37	$PrGa_{0.85}Mg_{0.15}O_{3-\delta}$	-4.81
$SrSc_{0.5}Al_{0.5}O_{3-\delta}$	-10.87	$Nd_{0.9}Ca_{0.1}Ga_{0.9}Mg_{0.1}O_{3-\delta}$	-4.79
$Yb_{0.9}Ca_{0.1}AlO_{3-\delta}$	-10.82	$La_{0.9}Sr_{0.1}InO_{3-\delta}$	-4.67
$SrSc_{0.4}Y_{0.1}Al_{0.5}O_{3-\delta}$	-10.27	$La_{0.5}Sr_{0.5}Ga_{0.7}Zr_{0.3}O_{3-\delta}$	-4.61
$SrSc_{0.45}Y_{0.05}Al_{0.5}O_{3-\delta}$	-10.11	$La_{0.9}Sr_{0.1}Ga_{0.9}Al_{0.1}O_{3-\delta}$	-4.44
$Nd_{0.9}Ba_{0.1}AlO_{3-\delta}$	-9.42	$La_{0.9}Sr_{0.1}ScO_{3-\delta}$	-4.37

化学式	*lnσ*	化学式	*lnσ*
$Sr_{0.8}Ba_{0.2}Sc_{0.5}Al_{0.5}O_{3-\delta}$	-8.98	$Pr_{0.9}Ca_{0.1}AlO_{3-\delta}$	-4.14
$SrSc_{0.5}Al_{0.45}Zn_{0.05}O_{3-\delta}$	-8.84	$CaTi_{0.95}Sc_{0.05}O_{3-\delta}$	-4.14
$SrSc_{0.5}Al_{0.45}Mg_{0.05}O_{3-\delta}$	-8.73	$CaTi_{0.85}Sc_{0.15}O_{3-\delta}$	-4.07
$SrSc_{0.5}Al_{0.35}Mg_{0.15}O_{3-\delta}$	-8.73	$La_{0.9}Sr_{0.1}Sc_{0.9}Mg_{0.1}O_{3-\delta}$	-3.96
$Nd_{0.9}Ca_{0.1}Al_{0.9}Zn_{0.1}O_{3-\delta}$	-8.57	$CaTi_{0.75}Sc_{0.25}O_{3-\delta}$	-3.91
$SrSc_{0.5}Al_{0.4}Zn_{0.1}O_{3-\delta}$	-8.57	$LaSc_{0.9}Mg_{0.1}O_{3-\delta}$	-3.91
$La_{0.5}Sr_{0.5}Ga_{0.55}Zr_{0.45}O_{3-\delta}$	-8.54	$Sm_{0.85}Ca_{0.15}AlO_{3-\delta}$	-3.86
$CaTiO_{3-\delta}$	-8.52	$Nd_{0.9}Ca_{0.1}Ga_{0.95}Mg_{0.05}O_{3-\delta}$	-3.85
$Nd_{0.9}Ba_{0.1}GaO_{3-\delta}$	-8.36	$La_{0.9}Sr_{0.1}Ga_{0.9}In_{0.1}O_{3-\delta}$	-3.85
$Nd_{0.9}Ca_{0.1}Al_{0.9}Mg_{0.1}O_{3-\delta}$	-8.11	$CaTi_{0.9}Sc_{0.1}O_{3-\delta}$	-3.82
$BaZr_{0.8}In_{0.2}O_{3-\delta}$	-8.04	$Sm_{0.78}Ca_{0.22}AlO_{3-\delta}$	-3.77
$SrSc_{0.5}Al_{0.4}Mg_{0.1}O_{3-\delta}$	-7.94	$La_{0.72}Yb_{0.08}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{3-\delta}$	-3.64
$Nd_{0.9}Ca_{0.1}Al_{0.9}Zr_{0.1}O_{3-\delta}$	-7.92	$PrGa_{0.95}Mg_{0.05}O_{3-\delta}$	-3.62
$Nd_{0.9}Sr_{0.1}AlO_{3-\delta}$	-7.71	$NdGa_{0.9}Mg_{0.1}O_{3-\delta}$	-3.49
$La_{0.7}Ca_{0.3}AlO_{3-\delta}$	-7.58	$Sm_{0.82}Ca_{0.18}AlO_{3-\delta}$	-3.47
$Nd_{0.9}Ca_{0.1}Al_{0.9}Be_{0.1}O_{3-\delta}$	-7.44	$Sm_{0.8}Ca_{0.2}AlO_{3-\delta}$	-3.35
$La_{0.9}Ca_{0.1}AlO_{3-\delta}$	-7.32	$PrGa_{0.75}Mg_{0.25}O_{3-\delta}$	-3.27
$CaTi_{0.75}Ga_{0.25}O_{3-\delta}$	-7.29	$La_{0.72}Y_{0.08}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{3-\delta}$	-3.13
$SrTiO_{3-\delta}$	-7.25	$La_{0.75}Sr_{0.25}Ga_{0.9}Mg_{0.1}O_{3-\delta}$	-3.11
$BaZr_{0.7}In_{0.3}O_{3-\delta}$	-7.21	$PrGa_{0.9}Mg_{0.1}O_{3-\delta}$	-2.99
$BaZr_{0.6}In_{0.4}O_{3-\delta}$	-7.14	$La_{0.72}Cd_{0.08}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{3-\delta}$	-2.97
$Sr_{0.9}Ba_{0.1}Sc_{0.6}Al_{0.3}Mg_{0.1}O_{3-\delta}$	-6.86	$Pr_{0.93}Ca_{0.07}Ga_{0.85}Mg_{0.15}O_{3-\delta}$	-2.9
$La_{0.9}Ba_{0.1}AlO_{3-\delta}$	-6.86	$Pr_{0.93}Sr_{0.07}Ga_{0.85}Mg_{0.15}O_{3-\delta}$	-2.67
$Nd_{0.9}Ca_{0.1}AlO_{3-\delta}$	-6.75	$La_{0.72}Sm_{0.08}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{3-\delta}$	-2.56
$Y_{0.9}Ca_{0.1}AlO_{3-\delta}$	-6.68	$La_{0.85}Sr_{0.15}Ga_{0.95}Mg_{0.05}O_{3-\delta}$	-2.51
$La_{0.5}Sr_{0.5}Ga_{0.6}Zr_{0.4}O_{3-\delta}$	-6.56	$La_{0.9}Sr_{0.1}Ga_{0.95}Mg_{0.05}O_{3-\delta}$	-2.42
$Nd_{0.9}Ca_{0.1}Al_{0.9}Ga_{0.1}O_{3-\delta}$	-6.52	$La_{0.8}Sr_{0.2}Ga_{0.95}Mg_{0.05}O_{3-\delta}$	-2.39
$BaIn_{0.8}Zr_{0.2}O_{3-\delta}$	-6.31	$La_{0.9}Sr_{0.1}Ga_{0.9}Mg_{0.1}O_{3-\delta}$	-2.36
$La_{0.9}Ca_{0.1}GaO_{3-\delta}$	-6.31	$La_{0.75}Sr_{0.25}Ga_{0.85}Mg_{0.15}O_{3-\delta}$	-2.26
$Nd_{0.9}Sr_{0.1}GaO_{3-\delta}$	-6.29	$La_{0.9}Sr_{0.1}Ga_{0.85}Mg_{0.15}O_{3-\delta}$	-2.15
$La_{0.9}Sr_{0.1}In_{0.9}Mg_{0.1}O_{3-\delta}$	-6.21	$La_{0.85}Sr_{0.15}Ga_{0.9}Mg_{0.1}O_{3-\delta}$	-2.11
$BaIn_{0.7}Zr_{0.3}O_{3-\delta}$	-6.17	$La_{0.8}Sr_{0.2}Ga_{0.85}Mg_{0.15}O_{3-\delta}$	-2.1
$La_{0.9}Sr_{0.1}AlO_{3-\delta}$	-6.01	$La_{0.85}Sr_{0.15}Ga_{0.8}Mg_{0.2}O_{3-\delta}$	-2.09

化学式	*lnσ*	化学式	*lnσ*
$Gd_{0.9}Ca_{0.1}AlO_{3-\delta}$	-5.99	$La_{0.9}Sr_{0.1}Ga_{0.75}Mg_{0.25}O_{3-\delta}$	-2.07
$CaTi_{0.8}Ga_{0.2}O_{3-\delta}$	-5.95	$La_{0.8}Sr_{0.2}Ga_{0.9}Mg_{0.1}O_{3-\delta}$	-2.06
$La_{0.9}Sr_{0.1}LuO_{3-\delta}$	-5.89	$La_{0.85}Sr_{0.15}Ga_{0.85}Mg_{0.15}O_{3-\delta}$	-2.03
$La_{0.9}Ba_{0.1}GaO_{3-\delta}$	-5.89	$La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{3-\delta}$	-2.03
$CaTi_{0.5}Al_{0.5}O_{3-\delta}$	-5.81	$La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.19}Co_{0.01}O_{3-\delta}$	-1.93
$BaIn_{0.6}Zr_{0.4}O_{3-\delta}$	-5.64	$La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.15}Co_{0.05}O_{3-\delta}$	-1.71
$BaIn_{0.9}Zr_{0.1}O_{3-\delta}$	-5.64	$La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.13}Co_{0.07}O_{3-\delta}$	-1.7
$CaTi_{0.9}Ga_{0.1}O_{3-\delta}$	-5.6	$La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.115}Co_{0.085}O_{3-\delta}$	-1.57
$Nd_{0.9}Ca_{0.1}GaO_{3-\delta}$	-5.48	$La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.17}Ni_{0.03}O_{3-\delta}$	-1.52
$CaTi_{0.85}Ga_{0.15}O_{3-\delta}$	-5.47	$La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.11}Co_{0.09}O_{3-\delta}$	-1.45
$CaTi_{0.95}Mg_{0.05}O_{3-\delta}$	-5.3	$La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.15}Ni_{0.05}O_{3-\delta}$	-1.45
$CaTi_{0.9}Al_{0.1}O_{3-\delta}$	-5.12	$La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.13}Ni_{0.07}O_{3-\delta}$	-1.43
$Sm_{0.9}Ca_{0.1}AlO_{3-\delta}$	-5.07	$La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.1}Ni_{0.1}O_{3-\delta}$	-1.31
$La_{0.9}Sr_{0.1}Al_{0.9}Mg_{0.1}O_{3-\delta}$	-4.96	$La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.05}Co_{0.15}O_{3-\delta}$	-1.24
$BaIn_{0.5}Zr_{0.5}O_{3-\delta}$	-4.95	$La_{0.7}Sr_{0.3}Ga_{0.7}Fe_{0.2}Mg_{0.1}O_{3-\delta}$	-1.24
$Nd_{0.9}Ca_{0.1}Al_{0.5}Ga_{0.5}O_{3-\delta}$	-4.93	$La_{0.8}Sr_{0.2}Ga_{0.8}Ni_{0.2}O_{3-\delta}$	0.04
$La_{0.5}Sr_{0.5}Ga_{0.75}Zr_{0.25}O_{3-\delta}$	-4.93		

表 S21 PSP 搜索的高氧离子电导率的钙钛矿化学式及其氧离子电导率预测值

Table S21: The chemical formula of the candidates with the corresponding predicted oxide ionic conductivity searched by PSP

化学式	*lnσ*	化学式	*lnσ*
$Pr_{0.7}Ba_{0.3}Ga_{0.87}Al_{0.13}O_{3-\delta}$	-1.385	$La_{0.8}Sr_{0.2}Ga_{0.801}Al_{0.199}O_{3-\delta}$	-1.313
$Pr_{0.78}Ba_{0.22}Ga_{0.805}Ti_{0.195}O_{3-\delta}$	-1.423	$La_{0.8}Sr_{0.2}Ga_{0.798}Ti_{0.202}O_{3-\delta}$	-1.430
$Pr_{0.77}Ba_{0.23}Ga_{0.805}Ti_{0.195}O_{3-\delta}$	-1.413	$La_{0.8}Sr_{0.2}Ga_{0.796}Ti_{0.204}O_{3-\delta}$	-1.423
$Pr_{0.765}Ba_{0.235}Ga_{0.808}Ti_{0.192}O_{3-\delta}$	-1.409	$La_{0.8}Sr_{0.2}Ga_{0.795}Al_{0.205}O_{3-\delta}$	-1.426
$Pr_{0.72}Ba_{0.28}Ga_{0.836}Ti_{0.164}O_{3-\delta}$	-1.412	$La_{0.8}Sr_{0.2}Ga_{0.793}Ti_{0.207}O_{3-\delta}$	-1.447
$Pr_{0.72}Ba_{0.28}Ga_{0.865}Al_{0.135}O_{3-\delta}$	-1.434	$La_{0.8}Sr_{0.2}Ga_{0.788}Ti_{0.212}O_{3-\delta}$	-1.395
$Pr_{0.72}Ba_{0.28}Ga_{0.855}Ti_{0.145}O_{3-\delta}$	-1.450	$La_{0.8}Sr_{0.2}Ga_{0.781}Ti_{0.219}O_{3-\delta}$	-1.355
$Pr_{0.72}Ba_{0.28}Ga_{0.844}Ti_{0.156}O_{3-\delta}$	-1.407	$La_{0.8}Sr_{0.2}Ga_{0.77}Ti_{0.23}O_{3-\delta}$	-1.398
$Pr_{0.72}Ba_{0.28}Ga_{0.841}Al_{0.159}O_{3-\delta}$	-1.429	$La_{0.8}Sr_{0.2}Ga_{0.775}Ti_{0.225}O_{3-\delta}$	-1.344
$Pr_{0.72}Ba_{0.28}Ga_{0.833}Ti_{0.167}O_{3-\delta}$	-1.420	$La_{0.8}Sr_{0.2}Ga_{0.81}Al_{0.19}O_{3-\delta}$	-1.327
$Pr_{0.72}Ba_{0.28}Ga_{0.829}Ti_{0.171}O_{3-\delta}$	-1.382	$La_{0.8}Sr_{0.2}Ga_{0.816}Al_{0.184}O_{3-\delta}$	-1.433

化学式	*lnσ*	化学式	*lnσ*
$Pr_{0.72}Ba_{0.28}Ga_{0.828}Ti_{0.172}O_{3-\delta}$	-1.436	$La_{0.81}Sr_{0.19}Ga_{0.808}Al_{0.192}O_{3-\delta}$	-1.444
$Pr_{0.72}Ba_{0.28}Ga_{0.795}Sc_{0.205}O_{3-\delta}$	-1.413	$La_{0.811}Sr_{0.189}Ga_{0.801}Al_{0.199}O_{3-\delta}$	-1.430
$Pr_{0.72}Ba_{0.28}Ga_{0.792}Sc_{0.208}O_{3-\delta}$	-1.411	$La_{0.806}Sr_{0.194}Ga_{0.811}Al_{0.189}O_{3-\delta}$	-1.421
$Pr_{0.72}Ba_{0.28}Ga_{0.785}Sc_{0.215}O_{3-\delta}$	-1.414	$La_{0.805}Sr_{0.195}Ga_{0.818}Al_{0.182}O_{3-\delta}$	-1.448
$Pr_{0.72}Ba_{0.28}Ga_{0.845}Al_{0.155}O_{3-\delta}$	-1.429	$La_{0.805}Sr_{0.195}Ga_{0.806}Ti_{0.194}O_{3-\delta}$	-1.405
$Pr_{0.71}Ba_{0.29}Ga_{0.8}Sc_{0.2}O_{3-\delta}$	-1.435	$La_{0.805}Sr_{0.195}Ga_{0.792}Ti_{0.208}O_{3-\delta}$	-1.448
$Pr_{0.71}Ba_{0.29}Ga_{0.871}Al_{0.129}O_{3-\delta}$	-1.376	$La_{0.805}Sr_{0.195}Ga_{0.78}Ti_{0.22}O_{3-\delta}$	-1.350
$Pr_{0.71}Ba_{0.29}Ga_{0.86}Ti_{0.14}O_{3-\delta}$	-1.443	$La_{0.805}Sr_{0.195}Ga_{0.786}Ti_{0.214}O_{3-\delta}$	-1.397
$Pr_{0.71}Ba_{0.29}Ga_{0.866}Al_{0.134}O_{3-\delta}$	-1.395	$La_{0.805}Sr_{0.195}Ga_{0.773}Ti_{0.227}O_{3-\delta}$	-1.400
$Pr_{0.71}Ba_{0.29}Ga_{0.865}Ti_{0.135}O_{3-\delta}$	-1.443	$La_{0.804}Sr_{0.196}Ga_{0.816}Al_{0.184}O_{3-\delta}$	-1.433
$Pr_{0.71}Ba_{0.29}Ga_{0.862}Ti_{0.138}O_{3-\delta}$	-1.436	$La_{0.804}Sr_{0.196}Ga_{0.805}Ti_{0.195}O_{3-\delta}$	-1.403
$Pr_{0.71}Ba_{0.29}Ga_{0.861}Ti_{0.139}O_{3-\delta}$	-1.432	$La_{0.803}Sr_{0.197}Ga_{0.8}Al_{0.2}O_{3-\delta}$	-1.387
$Pr_{0.71}B_{a0.29}Ga_{0.861}Al_{0.139}O_{3-\delta}$	-1.397	$La_{0.803}Sr_{0.197}Ga_{0.774}Ti_{0.226}O_{3-\delta}$	-1.343
$Pr_{0.71}Ba_{0.29}Ga_{0.85}Ti_{0.15}O_{3-\delta}$	-1.415	$La_{0.802}Sr_{0.198}Ga_{0.802}Ti_{0.198}O_{3-\delta}$	-1.425
$Pr_{0.71}Ba_{0.29}Ga_{0.859}Ti_{0.141}O_{3-\delta}$	-1.372	$La_{0.801}Sr_{0.199}Ga_{0.819}Al_{0.181}O_{3-\delta}$	-1.445
$Pr_{0.71}Ba_{0.29}Ga_{0.857}Ti_{0.143}O_{3-\delta}$	-1.426	$La_{0.801}Sr_{0.199}Ga_{0.797}Ti_{0.203}O_{3-\delta}$	-1.421
$Pr_{0.71}Ba_{0.29}Ga_{0.852}Al_{0.148}O_{3-\delta}$	-1.443	$La_{0.79}Sr_{0.21}Ga_{0.814}Al_{0.186}O_{3-\delta}$	-1.437
$Pr_{0.71}Ba_{0.29}Ga_{0.84}Ti_{0.16}O_{3-\delta}$	-1.416	$La_{0.79}Sr_{0.21}Ga_{0.806}Ti_{0.194}O_{3-\delta}$	-1.438
$Pr_{0.71}Ba_{0.29}Ga_{0.841}Ti_{0.159}O_{3-\delta}$	-1.417	$La_{0.79}Sr_{0.21}Ga_{0.801}Al_{0.199}O_{3-\delta}$	-1.399
$Pr_{0.71}Ba_{0.29}Ga_{0.837}Ti_{0.163}O_{3-\delta}$	-1.420	$La_{0.79}Sr_{0.21}Ga_{0.78}Ti_{0.22}O_{3-\delta}$	-1.415
$Pr_{0.71}Ba_{0.29}Ga_{0.831}Ti_{0.169}O_{3-\delta}$	-1.437	$La_{0.79}Sr_{0.21}Ga_{0.782}Ti_{0.218}O_{3-\delta}$	-1.415
$Pr_{0.71}Ba_{0.29}Ga_{0.82}Sc_{0.18}O_{3-\delta}$	-1.424	$La_{0.799}Sr_{0.201}Ga_{0.81}Ti_{0.19}O_{3-\delta}$	-1.446
$Pr_{0.71}Ba_{0.29}Ga_{0.829}Ti_{0.171}O_{3-\delta}$	-1.444	$La_{0.799}Sr_{0.201}Ga_{0.789}Ti_{0.211}O_{3-\delta}$	-1.397
$Pr_{0.71}Ba_{0.29}Ga_{0.823}Sc_{0.177}O_{3-\delta}$	-1.430	$La_{0.799}Sr_{0.201}Ga_{0.781}Ti_{0.219}O_{3-\delta}$	-1.357
$Pr_{0.71}Ba_{0.29}Ga_{0.79}Sc_{0.21}O_{3-\delta}$	-1.414	$La_{0.799}Sr_{0.201}Ga_{0.779}Ti_{0.221}O_{3-\delta}$	-1.348
$Pr_{0.71}Ba_{0.29}Ga_{0.795}Sc_{0.205}O_{3-\delta}$	-1.414	$La_{0.799}Sr_{0.201}Ga_{0.774}Ti_{0.226}O_{3-\delta}$	-1.397
$Pr_{0.71}Ba_{0.29}Ga_{0.785}Sc_{0.215}O_{3-\delta}$	-1.415	$La_{0.798}Sr_{0.202}Ga_{0.812}Al_{0.188}O_{3-\delta}$	-1.368
$Pr_{0.719}Ba_{0.281}Ga_{0.871}Al_{0.129}O_{3-\delta}$	-1.433	$La_{0.798}Sr_{0.202}Ga_{0.807}Ti_{0.193}O_{3-\delta}$	-1.405
$Pr_{0.719}Ba_{0.281}Ga_{0.869}Al_{0.131}O_{3-\delta}$	-1.405	$La_{0.798}Sr_{0.202}Ga_{0.805}Ti_{0.195}O_{3-\delta}$	-1.410
$Pr_{0.719}Ba_{0.281}Ga_{0.832}Ti_{0.168}O_{3-\delta}$	-1.375	$La_{0.798}Sr_{0.202}Ga_{0.79}Ti_{0.21}O_{3-\delta}$	-1.412
$Pr_{0.718}Ba_{0.282}Ga_{0.869}Al_{0.131}O_{3-\delta}$	-1.361	$La_{0.798}Sr_{0.202}Ga_{0.795}Ti_{0.205}O_{3-\delta}$	-1.425
$Pr_{0.718}Ba_{0.282}Ga_{0.856}Al_{0.144}O_{3-\delta}$	-1.435	$La_{0.797}Sr_{0.203}Ga_{0.809}Al_{0.191}O_{3-\delta}$	-1.393
$Pr_{0.716}Ba_{0.284}Ga_{0.86}Ti_{0.14}O_{3-\delta}$	-1.422	$La_{0.797}Sr_{0.203}Ga_{0.802}Al_{0.198}O_{3-\delta}$	-1.379

化学式	*lnσ*	化学式	*lnσ*
$Pr_{0.716}Ba_{0.284}Ga_{0.861}Ti_{0.139}O_{3-δ}$	-1.431	$La_{0.796}Sr_{0.204}Ga_{0.808}Ti_{0.192}O_{3-δ}$	-1.444
$Pr_{0.716}Ba_{0.284}Ga_{0.849}Al_{0.151}O_{3-δ}$	-1.386	$La_{0.795}Sr_{0.205}Ga_{0.807}Ti_{0.193}O_{3-δ}$	-1.448
$Pr_{0.716}Ba_{0.284}Ga_{0.798}Sc_{0.202}O_{3-δ}$	-1.418	$La_{0.795}Sr_{0.205}Ga_{0.779}Ti_{0.221}O_{3-δ}$	-1.413
$Pr_{0.715}Ba_{0.285}Ga_{0.86}Al_{0.14}O_{3-δ}$	-1.417	$La_{0.78}Sr_{0.22}Ga_{0.81}Al_{0.19}O_{3-δ}$	-1.413
$Pr_{0.715}Ba_{0.285}Ga_{0.859}Al_{0.141}O_{3-δ}$	-1.431	$La_{0.78}Sr_{0.22}Ga_{0.805}Ti_{0.195}O_{3-δ}$	-1.432
$Pr_{0.715}Ba_{0.285}Ga_{0.858}Ti_{0.142}O_{3-δ}$	-1.396	$La_{0.785}Sr_{0.215}Ga_{0.793}Ti_{0.207}O_{3-δ}$	-1.418
$Pr_{0.715}Ba_{0.285}Ga_{0.857}Al_{0.143}O_{3-δ}$	-1.433	$La_{0.784}Sr_{0.216}Ga_{0.808}Ti_{0.192}O_{3-δ}$	-1.434
$Pr_{0.715}Ba_{0.285}Ga_{0.855}Ti_{0.145}O_{3-δ}$	-1.416	$La_{0.783}Sr_{0.217}Ga_{0.811}Al_{0.189}O_{3-δ}$	-1.439
$Pr_{0.715}Ba_{0.285}Ga_{0.854}Al_{0.146}O_{3-δ}$	-1.401	$La_{0.781}Sr_{0.219}Ga_{0.801}Al_{0.199}O_{3-δ}$	-1.419
$Pr_{0.715}Ba_{0.285}Ga_{0.84}Ti_{0.16}O_{3-δ}$	-1.408	$La_{0.779}Sr_{0.221}Ga_{0.781}Ti_{0.219}O_{3-δ}$	-1.422
$Pr_{0.715}Ba_{0.285}Ga_{0.843}Ti_{0.157}O_{3-δ}$	-1.409	$La_{0.778}Sr_{0.222}Ga_{0.808}Ti_{0.192}O_{3-δ}$	-1.428
$Pr_{0.715}Ba_{0.285}Ga_{0.79}Sc_{0.21}O_{3-δ}$	-1.413	$La_{0.76}Ba_{0.24}Ga_{0.82}Sc_{0.18}O_{3-δ}$	-1.440
$Pr_{0.714}Ba_{0.286}Ga_{0.862}Ti_{0.138}O_{3-δ}$	-1.435	$La_{0.75}Ba_{0.25}Ga_{0.822}Sc_{0.178}O_{3-δ}$	-1.406
$Pr_{0.714}Ba_{0.286}Ga_{0.862}Al_{0.138}O_{3-δ}$	-1.395	$La_{0.74}Ba_{0.26}Ga_{0.89}Ti_{0.11}O_{3-δ}$	-1.445
$Pr_{0.714}Ba_{0.286}Ga_{0.821}Sc_{0.179}O_{3-δ}$	-1.436	$La_{0.74}Ba_{0.26}Ga_{0.88}Ti_{0.12}O_{3-δ}$	-1.388
$Pr_{0.713}Ba_{0.287}Ga_{0.8}Sc_{0.2}O_{3-δ}$	-1.432	$La_{0.74}Ba_{0.26}Ga_{0.884}Ti_{0.116}O_{3-δ}$	-1.402
$Pr_{0.713}Ba_{0.287}Ga_{0.858}Ti_{0.142}O_{3-δ}$	-1.407	$La_{0.74}Ba_{0.26}Ga_{0.873}Ti_{0.127}O_{3-δ}$	-1.372
$Pr_{0.713}Ba_{0.287}Ga_{0.832}Ti_{0.168}O_{3-δ}$	-1.429	$La_{0.74}Ba_{0.26}Ga_{0.866}Ti_{0.134}O_{3-δ}$	-1.426
$Pr_{0.713}Ba_{0.287}Ga_{0.82}Sc_{0.18}O_{3-δ}$	-1.421	$La_{0.74}Ba_{0.26}Ga_{0.865}Ti_{0.135}O_{3-δ}$	-1.414
$Pr_{0.712}Ba_{0.288}Ga_{0.872}Al_{0.128}O_{3-δ}$	-1.441	$La_{0.74}Ba_{0.26}Ga_{0.862}Ti_{0.138}O_{3-δ}$	-1.437
$Pr_{0.712}Ba_{0.288}Ga_{0.871}Al_{0.129}O_{3-δ}$	-1.376	$La_{0.74}Ba_{0.26}Ga_{0.84}Sc_{0.16}O_{3-δ}$	-1.430
$Pr_{0.712}Ba_{0.288}Ga_{0.853}Al_{0.147}O_{3-δ}$	-1.403	$La_{0.74}Ba_{0.26}Ga_{0.832}Sc_{0.168}O_{3-δ}$	-1.394
$Pr_{0.712}Ba_{0.288}Ga_{0.851}Al_{0.149}O_{3-δ}$	-1.394	$La_{0.74}Ba_{0.26}Ga_{0.831}Sc_{0.169}O_{3-δ}$	-1.395
$Pr_{0.712}Ba_{0.288}Ga_{0.849}Al_{0.151}O_{3-δ}$	-1.426	$La_{0.74}Ba_{0.26}Ga_{0.829}Sc_{0.171}O_{3-δ}$	-1.401
$Pr_{0.711}Ba_{0.289}Ga_{0.823}Sc_{0.177}O_{3-δ}$	-1.439	$La_{0.74}Ba_{0.26}Ga_{0.821}Sc_{0.179}O_{3-δ}$	-1.369
$Pr_{0.711}Ba_{0.289}Ga_{0.87}Al_{0.13}O_{3-δ}$	-1.362	$La_{0.745}Ba_{0.255}Ga_{0.86}Ti_{0.14}O_{3-δ}$	-1.433
$Pr_{0.711}Ba_{0.289}Ga_{0.86}Al_{0.14}O_{3-δ}$	-1.419	$La_{0.742}Ba_{0.258}Ga_{0.89}Ti_{0.11}O_{3-δ}$	-1.446
$Pr_{0.711}Ba_{0.289}Ga_{0.859}Ti_{0.141}O_{3-δ}$	-1.416	$La_{0.741}Ba_{0.259}Ga_{0.87}Al_{0.13}O_{3-δ}$	-1.416
$Pr_{0.711}Ba_{0.289}Ga_{0.856}Al_{0.144}O_{3-δ}$	-1.437	$La_{0.73}Ba_{0.27}Ga_{0.88}Ti_{0.12}O_{3-δ}$	-1.440
$Pr_{0.711}Ba_{0.289}Ga_{0.851}Al_{0.149}O_{3-δ}$	-1.434	$La_{0.73}Ba_{0.27}Ga_{0.875}Ti_{0.125}O_{3-δ}$	-1.424
$Pr_{0.711}Ba_{0.289}Ga_{0.792}Sc_{0.208}O_{3-δ}$	-1.412	$La_{0.739}Ba_{0.261}Ga_{0.871}Al_{0.129}O_{3-δ}$	-1.430
$Pr_{0.709}Ba_{0.291}Ga_{0.864}Al_{0.136}O_{3-δ}$	-1.439	$La_{0.738}Ba_{0.262}Ga_{0.885}Ti_{0.115}O_{3-δ}$	-1.416
$Pr_{0.705}Ba_{0.295}Ga_{0.859}Ti_{0.141}O_{3-δ}$	-1.432	$La_{0.737}Ba_{0.263}Ga_{0.863}Ti_{0.137}O_{3-δ}$	-1.445

化学式	*lnσ*	化学式	*lnσ*
$Pr_{0.69}Ba_{0.31}Ga_{0.86}Ti_{0.14}O_{3-\delta}$	-1.432	$La_{0.737}Ba_{0.263}Ga_{0.832}Sc_{0.168}O_{3-\delta}$	-1.398
$Pr_{0.69}Ba_{0.31}Ga_{0.862}Ti_{0.138}O_{3-\delta}$	-1.435	$La_{0.737}Ba_{0.263}Ga_{0.831}Sc_{0.169}O_{3-\delta}$	-1.398
$Pr_{0.69}Ba_{0.31}Ga_{0.859}Ti_{0.141}O_{3-\delta}$	-1.406	$La_{0.736}Ba_{0.264}Ga_{0.87}Al_{0.13}O_{3-\delta}$	-1.417
$Pr_{0.69}Ba_{0.31}Ga_{0.82}Sc_{0.18}O_{3-\delta}$	-1.399	$La_{0.735}Ba_{0.265}Ga_{0.88}Ti_{0.12}O_{3-\delta}$	-1.396
$Pr_{0.697}Ba_{0.303}Ga_{0.82}Sc_{0.18}O_{3-\delta}$	-1.450	$La_{0.735}Ba_{0.265}Ga_{0.887}Ti_{0.113}O_{3-\delta}$	-1.424
$Pr_{0.695}Ba_{0.305}Ga_{0.871}Al_{0.129}O_{3-\delta}$	-1.399	$La_{0.735}Ba_{0.265}Ga_{0.884}Ti_{0.116}O_{3-\delta}$	-1.410
$Pr_{0.685}Ba_{0.315}Ga_{0.864}Ti_{0.136}O_{3-\delta}$	-1.412	$La_{0.735}Ba_{0.265}Ga_{0.87}Ti_{0.13}O_{3-\delta}$	-1.434
$La_{0.8}Sr_{0.2}Ga_{0.818}Al_{0.182}O_{3-\delta}$	-1.447	$La_{0.735}Ba_{0.265}Ga_{0.876}Ti_{0.124}O_{3-\delta}$	-1.380
$La_{0.8}Sr_{0.2}Ga_{0.815}Al_{0.185}O_{3-\delta}$	-1.419	$La_{0.735}Ba_{0.265}Ga_{0.865}Ti_{0.135}O_{3-\delta}$	-1.422
$La_{0.8}Sr_{0.2}Ga_{0.813}Al_{0.187}O_{3-\delta}$	-1.436	$La_{0.735}Ba_{0.265}Ga_{0.84}Sc_{0.16}O_{3-\delta}$	-1.438
$La_{0.8}Sr_{0.2}Ga_{0.811}Al_{0.189}O_{3-\delta}$	-1.353	$La_{0.735}Ba_{0.265}Ga_{0.82}Sc_{0.18}O_{3-\delta}$	-1.425
$La_{0.8}Sr_{0.2}Ga_{0.809}Ti_{0.191}O_{3-\delta}$	-1.442	$La_{0.735}Ba_{0.265}Ga_{0.823}Sc_{0.177}O_{3-\delta}$	-1.372
$La_{0.8}Sr_{0.2}Ga_{0.808}Ti_{0.192}O_{3-\delta}$	-1.400		

表 S22 284 个高分子重读单元及其 DFT 计算禁带宽度值

Table S22: 284 repeating units and DFT calculated band gap values

重复单元	E_g/eV	重复单元	E_g /eV
CH_2-CO-NH-CS	2.691	NH-CO-CS-CO	1.441
CH_2-CS-C_6H_4-O	2.041	CO-C_6H_4-C_6H_4-C_6H_4	2.993
C_6H_4-C_6H_4-C_4H_2S-CS	1.807	CH_2-CH_2-C_4H_2S-O	4.186
CO-O-C_4H_2S-CS	1.918	NH-CS-CO-CS	1.512
C_6H_4-CS-C_4H_2S-O	1.930	CH_2-C_6H_4-CS-O	2.729
CO-C_6H_4-O-CS	2.772	CH_2-CO-C_4H_2S-CS	1.647
C_6H_4-O-CS-C_4H_2S	2.537	C_4H_2S-C_4H_2S-C_4H_2S-O	2.267
C_6H_4-C_4H_2S-C_6H_4-C_4H_2S	2.645	CO-C_4H_2S-C_6H_4-CS	1.708
NH-C_4H_2S-CO-C_4H_2S	2.678	CH_2-C_6H_4-NH-O	4.141
CH_2-NH-C_4H_2S-CS	2.063	NH-CS-NH-CS	2.491
NH-C_6H_4-CO-C_6H_4	3.042	CH_2-NH-CS-NH	4.019
NH-CO-CS-C_4H_2S	1.701	NH-C_4H_2S-C_4H_2S-CO	2.521
CO-C_6H_4-O-C_4H_2S	3.410	CH_2-C_4H_2S-CS-O	2.659
C_6H_4-CS-C_4H_2S-CS	1.332	NH-CO-C_4H_2S-O	3.567
CH_2-C_4H_2S-NH-C_4H_2S	3.092	CH_2-C_4H_2S-C_6H_4-O	3.375
CH_2-C_4H_2S-C_6H_4-C_4H_2S	2.872	C_6H_4-C_6H_4-C_6H_4-C_4H_2S	3.046

重复单元	E_g/eV	重复单元	E_g /eV
CH_2-NH-C_6H_4-CO	3.226	NH-C_6H_4-CO-O	3.667
CO-C_6H_4-C_4H_2S-CS	1.699	NH-C_4H_2S-CO-O	3.840
C_6H_4-C_6H_4-CS-O	2.623	NH-CS-NH-C_6H_4	3.426
CH_2-NH-C_4H_2S-C_6H_4	2.951	CO-CS-O-CS	1.532
NH-C_4H_2S-C_4H_2S-CH_2	2.919	CH_2-NH-CH_2-CS	2.141
CH_2-C_4H_2S-C_6H_4-CS	1.841	CH_2-CH_2-NH-C_6H_4	4.005
CH_2-NH-CS-C_6H_4	2.737	C_4H_2S-C_4H_2S-C_4H_2S-CS	1.686
CH_2-C_6H_4-C_4H_2S-C_6H_4	2.960	CH_2-C_6H_4-C_6H_4-O	3.823
NH-CO-C_4H_2S-C_6H_4	3.244	CH_2-CO-C_6H_4-CS	1.741
NH-C_4H_2S-NH-CS	3.123	CO-C_6H_4-C_6H_4-CS	1.800
CO-C_6H_4-C_4H_2S-O	2.590	CH_2-CH_2-CH_2-CS	2.315
NH-C_4H_2S-O-C_4H_2S	3.878	CH_2-C_6H_4-CH_2-O	4.867
CH_2-NH-CH_2-CO	3.842	CH_2-O-CO-O	6.933
NH-CO-NH-C_6H_4	4.455	NH-C_6H_4-CS-C_6H_4	1.924
CH_2-C_6H_4-NH-CS	2.960	CH_2-CO-C_6H_4-O	3.499
CH_2-CH_2-CH_2-O	6.863	CH_2-NH-C_4H_2S-NH	3.701
CH_2-CS-CH_2-O	2.411	CH_2-C_6H_4-CO-O	4.293
NH-C_6H_4-C_6H_4-O	3.619	CH_2-C_6H_4-CH_2-CS	2.354
CH_2-C_4H_2S-NH-CS	3.025	CH_2-C_6H_4-NH-C_6H_4	3.570
CH_2-C_6H_4-O-C_4H_2S	4.281	C_6H_4-C_4H_2S-C_6H_4-O	2.904
CH_2-CH_2-CO-C_6H_4	3.407	C_6H_4-C_4H_2S-O-CS	2.824
CO-C_4H_2S-C_4H_2S-CS	1.599	CH_2-C_4H_2S-C_4H_2S-CS	1.762
CH_2-C_6H_4-O-C_6H_4	4.132	CH_2-CO-CH_2-O	4.348
CO-C_4H_2S-C_6H_4-O	2.740	C_6H_4-C_4H_2S-C_4H_2S-C_4H_2S	2.321
CO-C_4H_2S-CO-O	2.930	CH_2-C_4H_2S-NH-O	3.964
CH_2-CS-C_4H_2S-O	2.028	CH_2-CO-C_6H_4-C_4H_2S	3.001
CH_2-O-C_4H_2S-C_6H_4	3.240	NH-CO-O-C_4H_2S	4.288
CH_2-C_4H_2S-CO-C_4H_2S	3.095	CH_2-C_4H_2S-CO-O	3.772
CO-C_6H_4-CO-O	2.979	CH_2-CS-C_6H_4-NH	2.063
CH_2-CH_2-CO-C_4H_2S	3.376	CO-O-C_6H_4-CS	1.932
CH_2-CO-CS-C_6H_4	1.754	NH-CO-C_4H_2S-CS	1.773
CH_2-CS-CO-O	1.599	NH-CO-O-CS	2.917
NH-C_4H_2S-NH-C_4H_2S	3.515	CH_2-NH-CS-CO	2.093

重复单元	E_g/eV	重复单元	E_g /eV
C_6H_4-CS-C_6H_4-CS	1.511	CH_2-CO-C_4H_2S-O	3.320
CH_2-C_6H_4-CH_2-C_6H_4	4.691	CH_2-CH_2-C_6H_4-O	4.351
CH_2-C_4H_2S-O-CS	3.061	CH_2-C_6H_4-CS-C_6H_4	1.889
CO-C_6H_4-C_6H_4-C_4H_2S	2.705	CO-C_6H_4-CO-C_6H_4	2.826
CH_2-CH_2-NH-C_4H_2S	3.931	CH_2-C_4H_2S-CH_2-O	4.313
CH_2-CH_2-CO-O	5.794	CH_2-NH-C_4H_2S-CO	2.987
CH_2-CO-CS-C_4H_2S	1.651	CH_2-NH-C_6H_4-NH	3.392
CH_2-NH-CH_2-NH	5.942	NH-CS-O-CS	2.557
C_6H_4-CS-C_4H_2S-C_4H_2S	1.728	CH_2-C_6H_4-O-CS	3.054
NH-CO-C_6H_4-CS	1.836	NH-CS-C_4H_2S-O	2.562
NH-CO-NH-CO	4.829	CO-C_6H_4-C_6H_4-O	2.965
C_4H_2S-C_4H_2S-O-CS	2.588	CH_2-NH-CH_2-C_4H_2S	4.226
NH-CS-NH-O	3.988	C_4H_2S-CS-O-CS	1.912
CO-O-C_4H_2S-O	4.016	CO-C_4H_2S-C_6H_4-C_4H_2S	2.505
CH_2-O-C_4H_2S-O	4.150	CO-C_4H_2S-C_4H_2S-C_4H_2S	2.080
NH-O-CO-O	6.731	CH_2-NH-CS-C_4H_2S	2.571
CH_2-CO-O-CS	2.705	NH-O-CS-O	4.333
CH_2-O-C_6H_4-O	3.859	CH_2-NH-CH_2-C_6H_4	4.318
NH-C_6H_4-NH-O	3.571	CH_2-C_6H_4-CO-C_4H_2S	3.144
CH_2-CH_2-C_6H_4-C_4H_2S	3.526	CH_2-O-CH_2-O	6.436
NH-C_4H_2S-CS-O	2.612	CO-C_6H_4-C_4H_2S-C_4H_2S	2.361
C_6H_4-C_6H_4-C_4H_2S-C_4H_2S	2.615	CH_2-CO-CS-O	2.161
NH-C_4H_2S-C_6H_4-C_4H_2S	2.584	NH-CO-CS-O	2.557
CO-C_4H_2S-C_4H_2S-O	2.360	CH_2-CO-CS-CO	1.278
NH-C_4H_2S-CO-CS	1.633	CH_2-NH-C_6H_4-C_4H_2S	3.176
NH-C_4H_2S-C_4H_2S-C_4H_2S	2.344	NH-CS-C_6H_4-CS	1.639
CH_2-CH_2-CH_2-C_6H_4	5.108	NH-C_6H_4-C_6H_4-CH_2	3.569
NH-C_4H_2S-O-CS	2.550	NH-CO-NH-CS	2.941
CH_2-NH-CS-O	4.240	NH-C_4H_2S-C_4H_2S-CS	1.764
CH_2-CO-O-C_4H_2S	4.022	NH-C_6H_4-NH-C_6H_4	3.313
CO-C_6H_4-CS-C_6H_4	1.753	NH-C_6H_4-NH-C_4H_2S	3.149
NH-CS-C_4H_2S-CS	1.614	CH_2-C_6H_4-C_6H_4-C_4H_2S	3.190
NH-CO-C_6H_4-C_4H_2S	3.238	CH_2-C_4H_2S-CS-C_4H_2S	1.802

重复单元	E_g/eV	重复单元	E_g /eV
NH-C_4H_2S-CS-C_4H_2S	1.882	CO-NH-CO-C_6H_4	3.710
C_6H_4-C_4H_2S-O-C_4H_2S	3.310	CH_2-CS-CO-CS	1.492
C_6H_4-C_6H_4-C_6H_4-CS	1.879	CH_2-CH_2-NH-CS	3.375
CH_2-C_4H_2S-CH_2-C_4H_2S	4.109	CH_2-C_4H_2S-C_4H_2S-O	2.817
CO-CS-CO-O	1.477	CH_2-CO-NH-C_4H_2S	4.130
CO-C_6H_4-C_4H_2S-C_6H_4	2.546	CH_2-CH_2-CO-CS	1.425
CH_2-CH_2-CH_2-CH_2	8.828	NH-C_6H_4-C_6H_4-C_4H_2S	2.930
NH-CO-C_6H_4-C_6H_4	3.656	CH_2-C_6H_4-C_4H_2S-CS	1.834
NH-CO-CS-C_6H_4	1.721	C_6H_4-O-CS-O	3.903
CO-C_6H_4-CS-C_4H_2S	1.787	CH_2-O-NH-CO	5.357
CH_2-CO-CH_2-CO	3.761	NH-C_6H_4-C_4H_2S-C_6H_4	2.753
CO-O-C_6H_4-O	4.193	C_6H_4-O-C_4H_2S-O	4.061
NH-CO-C_4H_2S-CO	3.029	NH-C_6H_4-O-C_4H_2S	3.606
CH_2-C_6H_4-C_4H_2S-C_4H_2S	2.737	CH_2-NH-CO-CS	1.827
CO-C_6H_4-CO-C_4H_2S	2.867	CH_2-NH-C_6H_4-O	3.538
CH_2-C_6H_4-CO-CS	1.735	C_6H_4-C_6H_4-C_6H_4-C_6H_4	3.307
CH_2-CH_2-C_6H_4-CS	1.965	CH_2-CO-NH-C_6H_4	4.296
NH-C_4H_2S-C_6H_4-CS	1.850	CH_2-CH_2-C_4H_2S-C_4H_2S	3.124
CH_2-NH-O-C_6H_4	4.520	CH_2-NH-CH_2-O	5.758
CH_2-C_6H_4-C_6H_4-C_6H_4	3.533	NH-C_6H_4-C_6H_4-C_6H_4	3.145
CH_2-O-NH-O	6.258	C_6H_4-CS-O-CS	1.914
CH_2-CH_2-C_4H_2S-CS	1.939	CO-C_4H_2S-CS-O	2.246
NH-CO-NH-C_4H_2S	4.069	NH-C_6H_4-C_4H_2S-C_4H_2S	2.587
CH_2-C_4H_2S-CH_2-CS	2.322	CH_2-CH_2-CH_2-NH	6.207
NH-CO-NH-O	5.284	CH_2-CO-NH-CO	4.232
CO-C_6H_4-CS-O	2.340	NH-CS-C_6H_4-O	2.700
CH_2-CH_2-O-NH	6.746	CO-C_4H_2S-CO-C_4H_2S	2.765
CH_2-CO-CH_2-C_4H_2S	3.997	NH-C_6H_4-O-CS	2.945
C_6H_4-O-C_6H_4-O	4.085	CH_2-C_4H_2S-CO-CS	1.532
CH_2-O-CS-O	3.958	CH_2-CO-O-C_6H_4	4.756
NH-CO-C_6H_4-O	4.072	C_4H_2S-C_4H_2S-C_4H_2S-C_4H_2S	2.019
C_4H_2S-O-C_4H_2S-O	4.103	CO-C_6H_4-O-C_6H_4	3.441
CH_2-NH-CO-C_6H_4	3.951	CH_2-CH_2-CH_2-C_4H_2S	4.506

重复单元	E_g/eV	重复单元	E_g /eV
CH_2-C_4H_2S-O-C_4H_2S	3.773	NH-CO-O-C_6H_4	4.926
CH_2-CO-O-CO	4.582	CO-C_4H_2S-O-CS	2.823
CH_2-CO-C_4H_2S-C_6H_4	3.020	C_6H_4-C_4H_2S-C_4H_2S-O	2.605
CH_2-CO-C_6H_4-CO	2.795	CH_2-CO-C_4H_2S-C_4H_2S	2.596
NH-C_4H_2S-C_4H_2S-O	2.834	CH_2-CO-CH_2-CS	2.174
C_6H_4-C_4H_2S-C_6H_4-CS	1.806	NH-C_6H_4-C_4H_2S-CS	1.856
CH_2-C_6H_4-CS-C_4H_2S	1.845	CH_2-C_4H_2S-C_4H_2S-C_4H_2S	2.328
C_6H_4-C_4H_2S-CS-C_4H_2S	1.740	NH-C_6H_4-CS-O	2.830
C_4H_2S-O-CS-O	3.820	NH-C_6H_4-CO-C_4H_2S	2.887
CH_2-CS-NH-O	3.256	CO-C_4H_2S-CO-CS	1.447
CH_2-C_6H_4-CH_2-C_4H_2S	4.409	NH-CS-CO-O	2.267
CO-O-CS-O	3.374	CH_2-CS-NH-CS	2.051
NH-C_6H_4-O-C_6H_4	3.875	C_6H_4-C_6H_4-C_4H_2S-O	2.951
CH_2-C_6H_4-CO-C_6H_4	3.186	CH_2-CO-C_4H_2S-CO	2.750
NH-CO-O-CO	5.163	CH_2-NH-CO-C_4H_2S	3.946
CO-C_4H_2S-CS-C_4H_2S	1.633	CH_2-C_6H_4-C_6H_4-CS	1.898
CH_2-CS-O-CS	2.214	CH_2-C_6H_4-NH-C_4H_2S	3.464
C_4H_2S-CS-C_4H_2S-O	1.860	CH_2-CO-C_6H_4-C_6H_4	3.215
CO-C_4H_2S-O-C_4H_2S	3.325	CH_2-CH_2-CS-O	3.309
C_6H_4-CS-C_6H_4-O	1.915	NH-C_4H_2S-CS-C_6H_4	1.964
NH-O-C_6H_4-O	3.916	CH_2-NH-O-C_4H_2S	4.294
CH_2-CO-CH_2-C_6H_4	4.257	C_6H_4-C_6H_4-C_6H_4-O	3.396
CH_2-NH-O-CS	3.231	NH-C_6H_4-CO-CS	1.760
CH_2-NH-C_4H_2S-O	3.881	CH_2-CH_2-C_6H_4-C_6H_4	4.020
CH_2-CS-C_4H_2S-CS	1.319	CH_2-CS-CH_2-CS	1.890
CO-C_6H_4-CO-CS	1.648	NH-C_6H_4-C_6H_4-CS	1.917
CH_2-CH_2-CH_2-CO	4.112	CH_2-NH-O-NH	5.865

表 S23 GMM 生成的 400 个虚拟样本及其 APS 参数

Table S23: 400 virtual samples and related APS parameters generated by GMM

结合强度/MPa	电流/A	电压/V	H_2 流速/L・min^{-1}	涂层厚度/μm
44.0817	640.9995	69.2988	4.9981	200
43.0779	640.9992	69.3005	4.9991	200

结合强度/MPa	电流/A	电压/V	H_2 流速/L・min^{-1}	涂层厚度/μm
44.2586	641.0013	69.3012	4.9995	200
42.4150	641.0001	69.2997	5.0005	200
45.2840	640.9993	69.2995	5.0009	200
28.7558	317.0005	64.9974	3.0003	400
30.9266	317.0010	65.0008	2.9998	400
31.0795	316.9988	64.9977	2.9980	400
31.1792	317.0023	64.9994	3.0009	400
29.2337	316.9999	65.0000	3.0001	400
31.8279	317.0003	65.0005	3.0007	400
31.4885	316.9998	64.9996	2.9995	400
30.7960	317.0004	64.9980	2.9999	400
29.8769	503.001	69.3009	4.9995	400
30.5272	503.0002	69.3019	5.0004	400
28.7079	503.0004	69.2988	5.0001	400
30.3132	502.9993	69.3007	4.9992	400
30.6571	503.0001	69.3015	5.0013	400
27.7909	503.0008	69.3010	4.9983	400
31.3886	502.9979	69.3006	5.0015	400
32.5995	503.0027	69.2989	5.0014	400
31.8907	503.0002	69.3007	5.0010	400
24.6319	520.0017	67.9991	5.0009	300
23.4812	519.9979	67.9988	5.0008	300
24.4193	520.0006	67.9987	5.0010	300
21.9762	519.9996	67.9991	5.0010	300
24.0895	519.9993	67.9991	5.0006	300
24.3513	520.0008	67.9998	5.0010	300
21.6935	519.9985	68.0006	5.0001	300
22.4808	519.9996	67.9990	4.9986	300
35.6751	664.9998	67.9985	6.0003	300
33.1503	665.0012	67.9996	6.0012	300
35.0482	665.0008	67.9994	6.0000	300
34.9945	665.0008	67.9994	5.9998	300
34.5622	665.0001	68.0001	6.0014	300
30.9414	665.0006	68.0000	6.0003	300
33.7359	665.0007	67.9987	5.9988	300
33.5073	665.0009	68.0011	5.9998	300
31.6889	665.0000	68.0011	6.0003	300
33.4840	665.0016	68.0004	5.9997	300
41.6065	317.0013	64.9993	2.9999	300
41.1682	317.0018	65.0002	3.0003	300
40.8115	317.0001	64.9995	2.9996	300
40.4448	317.0000	64.9996	2.9999	300
53.0654	617.0012	64.9987	3.0008	200

结合强度/MPa	电流/A	电压/V	H_2 流速/L·min^{-1}	涂层厚度/μm
55.0328	616.9995	64.9980	3.0009	200
53.7398	617.0001	64.9976	3.0014	200
55.6186	616.9991	64.9997	3.0021	200
52.1599	617.0008	65.0003	3.0010	200
54.1621	616.9999	65.0003	2.9998	200
32.2750	317.0005	64.9984	3.0005	400
28.6314	316.9998	65.0015	3.0005	400
30.4058	316.9997	65.0007	2.9985	400
31.4261	316.9999	65.0009	2.9999	400
31.5708	316.9993	65.0022	3.0006	400
40.7595	640.9996	69.2997	5.0015	200
43.4705	640.9987	69.2998	5.0005	200
20.8341	519.9988	67.9996	5.0001	300
23.4918	520.0004	68.0005	5.0001	300
22.9516	520.0009	68.0018	4.9994	300
23.1942	519.9993	68.0008	5.0001	300
23.9979	519.9993	68.0018	5.0014	300
23.8837	519.9984	67.9993	5.0009	300
23.7742	519.9999	67.9996	4.9995	300
23.3807	519.9997	68.0017	4.9990	300
23.7706	519.9980	68.0007	5.0012	300
22.5189	520.0018	68.0004	5.0000	300
23.4782	520.0001	67.9996	4.9997	300
21.6452	519.9994	67.9995	4.9995	300
24.8835	520.0011	68.0021	4.9983	300
22.8847	519.9979	67.9983	5.0003	300
22.8391	519.9995	67.9995	4.9979	300
34.7298	665.0005	67.9996	6.0005	300
35.2431	664.9989	67.9997	5.9992	300
31.4673	664.9989	67.9984	5.9998	300
31.4425	664.9999	68.0009	6.0012	300
37.2290	665.0015	68.0012	6.0015	300
33.4823	664.9982	67.9994	6.0003	300
33.7566	664.9988	68.0003	6.0002	300
43.4834	503.0012	69.3007	5.0019	200
43.1956	503.0004	69.3004	5.0023	200
44.2552	502.9987	69.3016	4.9990	200
42.6601	503.0014	69.3008	4.9993	200
44.8065	503.0010	69.3008	4.9994	200
41.4524	503.0005	69.2992	5.0034	200
42.3457	317.0001	64.9988	3.0007	300
40.5931	317.0001	65.0014	2.9997	300
41.8046	316.9994	65.0011	3.0001	300

结合强度/MPa	电流/A	电压/V	H_2 流速/L・min^{-1}	涂层厚度/μm
39.4489	316.9981	65.0007	2.9999	300
40.4981	317.0005	65.0010	3.0008	300
41.5466	316.9988	64.9993	2.9998	300
40.5588	317.0009	65.0012	3.0005	300
40.0070	317.0003	65.0010	2.9999	300
42.2277	316.9991	65.0004	3.0002	300
49.7651	616.9995	65.0007	2.9994	200
54.4662	617.0021	64.9989	3.0016	200
51.1790	617.0004	65.0010	3.0011	200
52.2378	617.0010	64.9998	2.9992	200
53.1824	617.0010	65.0000	3.0003	200
51.2631	616.9996	64.9994	3.0002	200
34.2177	662.5482	67.5614	5.7957	300
30.3303	670.5705	68.9979	6.4640	300
34.8572	661.2322	67.3239	5.6863	300
35.2409	660.4370	67.1824	5.6177	300
32.1907	666.7260	68.3081	6.1433	300
36.5659	657.7039	66.6933	5.3889	300
30.8427	669.5142	68.8065	6.3768	300
32.0648	666.9944	68.3573	6.1663	300
28.5989	674.1435	69.6384	6.7587	300
32.7650	665.5492	68.0997	6.0444	300
34.9455	661.0458	67.2934	5.6712	300
35.2972	660.3150	67.1607	5.6095	300
31.5901	667.9710	68.5320	6.2482	300
36.5101	657.8169	66.7136	5.4016	300
33.4171	664.2019	67.8571	5.9337	300
29.5231	319.9440	65.5279	3.2465	400
31.8414	315.1632	64.6718	2.8474	400
31.0302	316.8347	64.9697	2.9883	400
27.6681	323.7790	66.2144	3.5638	400
30.6906	317.5368	65.0968	3.0443	400
32.2110	314.3986	64.5337	2.7816	400
27.9022	323.2883	66.1277	3.5256	400
31.7902	315.2640	64.6900	2.8559	400
20.7388	525.3878	68.9657	5.4499	300
21.7936	523.2124	68.5752	5.2659	300
19.6957	527.5349	69.3507	5.6283	300
27.1998	512.0578	66.5772	4.3383	300
22.3086	522.1496	68.3847	5.1781	300
27.4365	511.5653	66.4883	4.2977	300
45.4154	632.2972	67.7412	4.2751	200
43.0835	637.1140	68.6033	4.6760	200

结合强度/MPa	电流/A	电压/V	H_2 流速/L・min^{-1}	涂层厚度/μm
50.9428	620.8947	65.6977	3.3251	200
43.3077	502.7795	69.2606	4.9812	200
39.2926	511.0632	70.7464	5.6726	200
48.1596	492.7621	67.4663	4.1469	200
42.5441	313.3412	64.3431	2.6954	300
39.8271	318.9418	65.3496	3.1647	300
38.6564	321.3619	65.7800	3.3641	300
43.0203	312.3578	64.1681	2.6132	300
43.9270	310.4832	63.8319	2.4570	300
41.7762	314.9253	64.6283	2.8268	300
41.4445	315.6113	64.7527	2.8859	300
28.9982	505.6869	69.7811	5.2255	400
30.1403	503.3311	69.3576	5.0281	400
25.9974	511.8791	70.8911	5.7393	400
31.1890	501.1628	68.9708	4.8459	400
31.9566	499.5806	68.6872	4.7137	400
34.3191	494.7071	67.8143	4.3064	400
23.9065	516.1931	71.6618	6.0997	400
32.2120	499.0555	68.5915	4.6715	400
32.5610	666.8096	68.3235	6.1501	300
32.6044	666.6325	68.2915	6.1369	300
31.5540	670.6819	69.0167	6.4730	300
34.2684	660.2175	67.1440	5.6003	300
29.7502	677.6357	70.2640	7.0515	300
31.7328	669.9988	68.8970	6.4163	300
33.9740	661.3639	67.3488	5.6973	300
35.9217	653.8616	66.0034	5.0711	300
36.4411	651.8611	65.6457	4.9060	300
34.9644	657.5454	66.6639	5.3782	300
33.0056	665.0945	68.0167	6.0090	300
31.7928	313.7546	64.4181	2.7284	400
28.7207	325.5836	66.5360	3.7160	400
30.5732	318.4519	65.2598	3.1210	400
29.3334	323.2252	66.1153	3.5168	400
31.0687	316.5413	64.9170	2.9623	400
31.2377	315.8883	64.8017	2.9063	400
31.4927	314.9122	64.6260	2.8251	400
30.1373	320.1273	65.5591	3.2596	400
43.0578	503.5402	69.3961	5.0464	200
41.1093	511.0589	70.7424	5.6718	200
42.8619	504.3052	69.5346	5.1084	200
41.5470	509.3665	70.4402	5.5299	200
42.7496	504.7325	69.6109	5.1430	200

结合强度/MPa	电流/A	电压/V	H_2 流速/L・min^{-1}	涂层厚度/μm
43.5759	501.5588	69.0416	4.8794	200
41.1995	510.7069	70.6800	5.6418	200
46.2462	491.2580	67.1949	4.0215	200
44.8723	496.5572	68.1468	4.4622	200
42.5905	505.3542	69.7200	5.1962	200
42.7479	504.7433	69.6098	5.1459	200
20.8046	529.8086	69.7571	5.8176	300
23.1461	520.7810	68.1394	5.0663	300
21.2015	528.2783	69.4837	5.6873	300
22.7497	522.3127	68.4143	5.1919	300
25.0407	513.4920	66.8342	4.4574	300
24.0030	517.4805	67.5497	4.7901	300
46.7535	640.4078	69.1919	4.9506	200
50.7315	625.0834	66.4500	3.6751	200
50.1601	627.2809	66.8409	3.8573	200
47.9758	635.6887	68.3519	4.5566	200
52.8155	617.0538	65.0114	3.0043	200
30.6638	501.5935	69.0490	4.8802	400
28.4530	510.1188	70.5759	5.5951	400
29.4975	506.1004	69.8558	5.2580	400
39.5202	321.8112	65.8627	3.4016	300
39.3084	322.6325	66.0083	3.4686	300
42.5706	310.0573	63.7576	2.4224	300
39.6702	321.2408	65.7591	3.3529	300
41.1902	315.3745	64.7088	2.8658	300
44.0300	304.4390	62.7499	1.9535	300
32.5117	317.0012	65.0010	2.9981	400
28.9660	316.9976	65.0020	2.9993	400
29.8990	316.9995	65.0013	3.0000	400
30.5737	317.0009	64.9994	3.0007	400
29.8925	316.9983	65.0011	3.0011	400
32.4183	317.0015	64.9989	3.0002	400
32.2215	316.9999	65.0006	2.9985	400
32.8574	316.9996	64.9990	3.0012	400
30.4274	317.0000	65.0006	3.0009	400
31.914	316.9999	64.9998	3.0005	400
30.5567	316.9991	64.9981	3.0002	400
30.7230	317.0017	65.0009	2.9989	400
30.4443	316.9995	64.9988	3.0000	400
51.9602	617.0012	65.0006	3.0013	200
51.6783	617.0016	64.9998	2.9998	200
50.8285	617.0003	65.0011	3.0005	200
50.1888	616.9988	65.0001	3.0021	200

结合强度/MPa	电流/A	电压/V	H_2 流速/L・min^{-1}	涂层厚度/μm
52.4762	616.9998	64.9997	2.9995	200
32.7309	503.0012	69.3001	4.9992	400
28.6437	503.0008	69.2985	5.0027	400
33.0430	503.0009	69.3008	5.0000	400
30.0791	503.0006	69.3006	4.9997	400
31.1330	503.0014	69.3008	4.9996	400
29.0252	502.9998	69.3003	5.0010	400
30.4681	503.0004	69.3007	4.9996	400
29.0757	502.9996	69.3010	5.0003	400
31.2320	503.0016	69.2988	5.0002	400
44.1315	502.9997	69.3019	4.9988	200
43.6223	502.9996	69.2987	5.0000	200
41.1338	503.0017	69.2990	5.0002	200
40.8660	502.9996	69.3021	5.0016	200
43.4637	502.9997	69.2995	5.0000	200
41.4376	502.9989	69.3018	5.0006	200
40.5547	503.0018	69.3012	5.0002	200
42.2831	503.0010	69.3012	5.0002	200
45.4795	502.9999	69.2968	4.9999	200
34.3591	665.0015	68.0018	5.9998	300
34.9782	664.9997	67.9994	5.9996	300
33.3174	664.9986	67.9990	5.9982	300
33.2613	664.9989	67.9997	6.0003	300
32.8849	665.0012	67.9995	6.0015	300
40.2725	317.0009	65.0005	3.0002	300
41.3895	316.9997	65.0011	2.9978	300
42.4313	317.0009	64.9982	3.0000	300
42.9913	316.9965	65.0005	2.9979	300
38.7601	316.9983	64.9999	3.0007	300
40.9593	316.9998	65.0007	3.0007	300
42.5998	316.9996	65.0001	3.0005	300
41.2976	641.0026	69.3001	4.9986	200
43.4614	641.0012	69.3002	5.0005	200
51.0123	617.0000	64.9982	2.9994	200
52.7283	617.0000	65.0027	3.0009	200
52.4600	616.9993	65.0004	2.9995	200
52.3568	617.0021	65.0015	3.0002	200
53.7234	617.0002	64.9995	2.9978	200
54.5434	617.0005	64.9991	2.9978	200
38.5490	316.9997	64.9993	2.9986	300
40.8951	316.9990	64.9981	2.9987	300
40.1907	317.0014	64.9991	3.0002	300
40.1921	316.9989	64.9987	3.0000	300

结合强度/MPa	电流/A	电压/V	H_2 流速/L・min^{-1}	涂层厚度/μm
40.1086	317.0003	64.9978	2.9981	300
39.8727	317.0023	64.9981	2.9981	300
38.5573	316.9982	65.0008	3.0005	300
41.0864	317.0000	65.0010	3.0007	300
42.0984	317.0001	65.0004	2.9995	300
39.6358	317.0007	64.9995	3.0009	300
41.3408	317.0005	65.0006	3.0006	300
29.0254	503.0009	69.3000	4.9980	400
31.4068	503.0010	69.3004	4.9984	400
31.4717	503.0013	69.3009	5.0017	400
29.0862	503.0005	69.3012	5.0012	400
33.3520	502.9993	69.3009	4.9999	400
30.7504	502.9979	69.2999	4.9976	400
30.7121	502.9997	69.3012	4.9977	400
38.8716	503.0011	69.2992	4.9995	200
44.1711	502.9994	69.3007	5.0009	200
42.5385	503.0021	69.2990	5.0003	200
42.8611	503.0010	69.3007	5.0006	200
43.8163	503.0002	69.3007	4.9983	200
43.3795	503.0017	69.2974	4.9994	200
41.9027	503.0004	69.2999	4.9984	200
44.7915	502.9997	69.2998	4.9998	200
44.4960	503.0004	69.2993	5.0019	200
43.5709	503.0009	69.3004	4.9990	200
44.5054	503.0006	69.3005	4.9998	200
25.0572	519.9993	67.9989	5.0001	300
24.6308	519.9985	68.0007	4.9999	300
24.6019	520.0015	68.0009	4.9983	300
26.1934	519.9992	67.9985	4.9998	300
25.7477	520.0008	68.0019	4.9993	300
22.7984	519.9991	67.9997	4.9998	300
30.6312	316.9986	65.0007	2.9983	400
43.6082	641.0002	69.3001	5.0007	200
45.6074	640.9987	69.2995	5.0001	200
44.1741	641.0005	69.2991	5.0006	200
42.9883	640.9991	69.2995	4.9999	200
45.2294	640.9997	69.2978	5.0005	200
43.3729	641.0003	69.2990	5.0012	200
41.9219	641.0010	69.2989	5.0004	200
41.3191	641.0001	69.299	4.9995	200
53.5511	616.9995	64.9994	3.0007	200
53.8831	617.0016	65.0013	2.9995	200
55.9450	617.0004	64.9995	2.9997	200

结合强度/MPa	电流/A	电压/V	H_2 流速/L・min^{-1}	涂层厚度/μm
51.3989	617.0018	65.0010	3.0004	200
55.9015	617.0000	65.0008	2.9993	200
51.2026	616.9995	65.0002	2.9994	200
53.0625	617.0004	65.0008	3.0002	200
54.1021	616.9984	65.0003	3.0003	200
54.2423	616.9986	64.9992	3.0010	200
30.7328	317.0007	64.9998	2.9987	400
31.5578	316.9993	65.0002	2.9999	400
29.7320	317.0012	64.9994	2.9997	400
32.4214	317.0007	65.0004	2.9991	400
31.0192	316.9994	64.9989	3.0003	400
31.5187	316.9990	65.0003	2.9997	400
30.9732	502.9997	69.2995	4.9978	400
31.9578	503.0007	69.3002	4.9985	400
30.4410	502.9984	69.3010	4.9996	400
31.0847	503.0021	69.3007	4.9994	400
30.4804	502.9994	69.3013	5.0002	400
30.8195	502.9995	69.3001	4.9990	400
29.4819	503.0004	69.2990	4.9996	400
28.7762	503.0012	69.2997	5.0001	400
33.5909	503.0000	69.3004	5.0004	400
31.9001	503.0008	69.2986	5.0003	400
31.3886	502.9995	69.3016	5.0003	400
42.2168	502.9992	69.3006	4.9991	200
44.1314	502.9990	69.3007	4.9997	200
41.0202	502.9999	69.2978	4.9990	200
44.2527	503.0010	69.3014	4.9989	200
41.9073	502.9988	69.2981	5.0014	200
44.9328	502.9999	69.2982	5.0006	200
43.3108	502.9996	69.299	4.9988	200
44.4737	502.9996	69.3001	5.0006	200
45.1654	502.9980	69.3006	5.0011	200
42.9331	503.0001	69.3002	4.9999	200
32.1774	664.9991	67.9983	6.0009	300
32.6768	665.0002	67.9996	5.9982	300
30.7743	665.0016	67.9995	6.0012	300
33.1528	665.0000	67.9980	5.9998	300
35.1260	664.9999	68.0007	5.9994	300
21.8358	520.0002	68.0003	5.0011	300
24.9826	519.9988	67.9995	5.0006	300
24.1903	519.9987	68.0013	4.9986	300
23.4032	519.9990	67.9996	5.0002	300
24.7379	519.9993	68.0005	4.9988	300

结合强度/MPa	电流/A	电压/V	H_2 流速/L・min^{-1}	涂层厚度/μm
24.4303	519.9987	67.9995	5.0002	300
44.1962	640.9995	69.2992	5.0004	200
42.2185	641.0001	69.2996	5.0006	200
45.4463	641.0015	69.3005	4.9993	200
44.1439	641.0006	69.3007	5.0008	200
44.1607	640.9980	69.2999	4.9975	200
45.8665	640.9984	69.3001	4.9988	200
44.3251	641.0004	69.3026	5.0004	200
42.6104	316.9986	65.0000	3.0006	300
39.9180	317.0019	64.9997	3.0007	300
44.4096	317.0002	64.9991	2.9980	300
43.0358	316.9986	65.0010	2.9996	300
42.3085	316.9985	64.9994	2.9995	300
41.5329	316.9996	65.0002	3.0014	300
38.6270	317.0005	65.0012	3.0000	300
41.5336	317.0004	65.0002	3.0001	300
25.1858	519.9987	68.0025	5.0003	300
22.4711	520.0018	68.0020	4.9997	300
25.7054	519.9977	67.9989	5.0000	300
22.9594	520.0010	68.0007	4.9992	300
22.4064	519.9991	68.0003	5.0012	300
23.5074	520.0006	68.0009	5.0005	300
33.4169	664.9996	68.0004	6.0003	300
32.5526	664.9997	67.9999	5.9983	300
33.2946	665.0005	68.0020	6.0001	300
32.1656	664.9986	67.9986	5.9997	300
34.1750	664.9994	67.9985	5.9997	300
33.2705	665.0003	67.9998	6.0002	300
33.7396	665.0002	67.9999	6.0015	300
33.7023	664.9989	68.0003	5.9994	300
32.3414	664.9988	67.9999	6.0008	300
44.4754	502.9993	69.2985	5.0007	200
45.6420	503.0004	69.3000	4.9994	200
43.4198	503.0001	69.2999	4.9998	200
43.1737	502.9983	69.3023	5.0004	200
40.7342	502.9993	69.3001	5.0007	200
42.4076	503.0000	69.3007	5.0002	200
42.0911	503.0014	69.2998	5.0021	200
42.9336	503.0007	69.3002	4.9987	200
40.8400	502.9978	69.2999	4.9995	200
43.1017	503.0015	69.3012	4.9989	200
43.1239	503.0004	69.2998	5.0008	200
28.4511	503.0015	69.2997	5.0008	400

结合强度/MPa	电流/A	电压/V	H_2 流速/L・min^{-1}	涂层厚度/μm
29.9719	503.0004	69.2990	4.9995	400
30.2650	502.9992	69.2992	4.9997	400
29.5692	502.9991	69.2988	5.0008	400
29.8095	502.9994	69.3000	4.9998	400
28.4760	502.9999	69.2978	4.9990	400
29.7915	503.0004	69.3003	5.0006	400
51.4407	616.9990	65.0004	2.9984	200
53.0423	616.9991	64.9990	2.9988	200
51.5460	616.9990	64.9994	2.9997	200
51.0616	616.9985	64.9995	3.0007	200
54.8993	616.9994	65.0000	2.9992	200

表 S24：30 次随机划分 LOOCV、10 折交叉验证和独立测试的 R、RMSE 以及相应的平均值和标准偏差（σ）

Table S3: The R, RMSE with corresponding average and standard deviation values (σ) of LOOCV, 10-fold CV and independent test based on 30 times of random divided training set and test set at the ratio of 4:1

NO	LOOCV		10-fold CV		Independent test	
	R	RMSE	R	RMSE	R	RMSE
1	0.988	1.292	0.988	1.295	0.990	1.340
2	0.987	1.385	0.988	1.320	0.990	1.228
3	0.989	1.295	0.989	1.289	0.990	1.308
4	0.990	1.264	0.990	1.263	0.986	1.413
5	0.990	1.254	0.989	1.313	0.987	1.370
6	0.989	1.303	0.989	1.331	0.988	1.244
7	0.988	1.332	0.988	1.352	0.992	1.095
8	0.989	1.253	0.989	1.279	0.989	1.367
9	0.989	1.304	0.988	1.322	0.990	1.267
10	0.989	1.317	0.989	1.307	0.987	1.337
11	0.988	1.381	0.988	1.384	0.992	1.064
12	0.988	1.340	0.988	1.343	0.991	1.185
13	0.988	1.309	0.988	1.299	0.987	1.466
14	0.989	1.300	0.989	1.292	0.987	1.276

NO	LOOCV		10-fold CV		Independent test	
	R	RMSE	R	RMSE	R	RMSE
15	0.989	1.315	0.989	1.290	0.982	1.279
16	0.99	1.282	0.990	1.277	0.979	1.379
17	0.988	1.294	0.988	1.313	0.991	1.197
18	0.988	1.389	0.988	1.367	0.991	1.103
19	0.988	1.313	0.988	1.304	0.990	1.266
20	0.989	1.253	0.989	1.251	0.985	1.470
21	0.988	1.315	0.988	1.296	0.990	1.355
22	0.990	1.230	0.989	1.268	0.984	1.518
23	0.989	1.338	0.989	1.327	0.991	1.487
24	0.989	1.271	0.989	1.289	0.989	1.342
25	0.989	1.282	0.989	1.289	0.985	1.381
26	0.989	1.290	0.989	1.280	0.988	1.411
27	0.988	1.373	0.988	1.352	0.991	1.121
28	0.989	1.281	0.989	1.292	0.989	1.384
29	0.988	1.315	0.988	1.302	0.990	1.321
30	0.988	1.320	0.988	1.314	0.989	1.314
均值	0.989	1.306	0.989	1.307	0.988	1.310
σ	0.000745	0.0387	0.000605	0.0298	0.00292	0.114