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**博士学位论文**

**SHANGHAI UNIVERSITY DOCTORAL DISSERTATION**

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| --- | --- |
| **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/ |
| 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/ |
| 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 个物理性质。 | https://www.paulingfile.com/ |
| 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 |
| 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。 |
| 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。 |
| 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 |
| 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 |
| --- | --- | --- | --- | --- |
| BaCu0.33Nb0.67O3 | 0 |  | SrFe0.5Ta0.5O3 | 0 |
| SrCu0.33Nb0.67O3 | 0 |  | PbNi0.5Ti0.25W0.25O3 | 0 |
| SrCu0.33Ta0.67O3 | 0 |  | PbMn0.5Nb0.5O3 | 0 |
| PbCd0.33Nb0.67O3 | 0 |  | Sr0.5La0.5Cu0.5Sb0.5O3 | 0 |
| BaBi0.5Nb0.5O3 | 0 |  | Sr0.5La0.5Cu0.33Sb0.67O3 | 0 |
| BaBi0.5Ta0.5O3 | 0 |  | Sr0.5La0.5Cu0.5Ta0.5O3 | 0 |
| TlNa0.2W0.8O3 | 0 |  | SrNi0.5Re0.5O3 | 0 |
| TlCd0.25W0.75O3 | 0 |  | SrFe0.5Re0.5O3 | 0 |
| TlY0.33W0.67O3 | 0 |  | PbMn0.5W0.5O3 | 1 |
| TlGd0.33W0.67O3 | 0 |  | PbMn0.5Re0.5O3 | 1 |
| TlDy0.33W0.67O3 | 0 |  | PbMn0.5Re0.5O3 | 1 |
| TlFe0.33W0.67O3 | 0 |  | PbMn0.5W0.5O3 | 1 |
| TlTi0.33W0.67O3 | 0 |  | PbCd0.5W0.5O3 | 1 |
| NaTaO3 | 0 |  | NaNbO3 | 1 |
| SrTiO3 | 0 |  | PbMg0.5W0.5O3 | 1 |
| BaTiO3 | 0 |  | PbCo0.5W0.5O3 | 1 |
| PbTiO3 | 0 |  | PbIn0.5Nb0.5O3 | 1 |
| PbSc0.5Nb0.5O3 | 0 |  | PbYb0.5Nb0.5O3 | 1 |
| PbSc0.5Ta0.5O3 | 0 |  | PbLu0.5Nb0.5O3 | 1 |
| PbFe0.5Ta0.5O3 | 0 |  | PbYb0.5Ta0.5O3 | 1 |
| PbZn0.33Nb0.67O3 | 0 |  | PbZn0.5W0.5O3 | 1 |
| PbCo0.33Nb0.67O3 | 0 |  | PbNi0.5W0.5O3 | 1 |
| PbNi0.33Nb0.67O3 | 0 |  | PbBi0.5Nb0.5O3 | 1 |
| PbMg0.33Ta0.67O3 | 0 |  | PbCd0.25Mn0.25Nb0.5O3 | 1 |
| PbCo0.33Ta0.67O3 | 0 |  | PbCd0.25Ti0.25Ta0.5O3 | 1 |
| PbNi0.33Ta0.67O3 | 0 |  | PbSnO3 | 1 |
| PbFe0.67W0.33O3 | 0 |  | PbZr0.94Ti0.06O3 | 1 |
| DyCrO3 | 0 |  | SrMn0.5Re0.5O3 | 1 |
| YbCrO3 | 0 |  | BaMn0.5Re0.5O3 | 1 |
| LuCrO3 | 0 |  | PbFe0.5Re0.5O3 | 1 |
| PrCrO3 | 0 |  | PbCo0.5Re0.5O3 | 1 |
| PbCo0.5W0.5O3 | 0 |  | PbNi0.5Re0.5O3 | 1 |
| CdFe0.5Nb0.5O3 | 0 |  | BaCd0.33Nb0.67O3 | 1 |
| CdSc0.5Nb0.5O3 | 0 |  | BaMg0.33Nb0.67O3 | 1 |
| CdMg0.33Nb0.67O3 | 0 |  | SrCd0.33Nb0.67O3 | 1 |
| PbCr0.5Nb0.5O3 | 0 |  | BaFe0.5Nb0.5O3 | 1 |
| PbLi0.25Sc0.25W0.5O3 | 0 |  | BaSc0.5Nb0.5O3 | 1 |
| PbLi0.25Fe0.25W0.5O3 | 0 |  | CaCr0.5Nb0.5O3 | 1 |
| PbLi0.25In0.25W0.5O3 | 0 |  | NdMg0.5Ti0.5O3 | 1 |
| PbLi0.25Tb0.25W0.5O3 | 0 |  | Na0.5La0.5TiO3 | 1 |
| PbLi0.25Yb0.25W0.5O3 | 0 |  | K0.5La0.5TiO3 | 1 |
| PbLi0.25Gd0.25W0.5O3 | 0 |  | Na0.5Nd0.5TiO3 | 1 |
| PbLi0.25La0.25W0.5O3 | 0 |  | CdSnO3 | 1 |
| PbLi0.25Sm0.25W0.5O3 | 0 |  | CaZrO3 | 1 |
| PbNa0.25Y0.25W0.5O3 | 0 |  | CaSnO3 | 1 |
| PbCd0.45Nb0.22W0.33O3 | 0 |  | CaMoO3 | 1 |
| PbSc0.25Cr0.25W0.5O3 | 0 |  | CaRuO3 | 1 |
| PbMg0.25Mn0.25W0.5O3 | 0 |  | CaTiO3 | 1 |
| PbCd0.25Mn0.25W0.5O3 | 0 |  | CdPbO3 | 1 |
| PbCo0.25Mn0.25W0.5O3 | 0 |  | CdZrO3 | 1 |
| PbNi0.25Mn0.25W0.5O3 | 0 |  | SrPbO3 | 1 |
| PbNi0.25Mn0.25Nb0.5O3 | 0 |  | SrSnO3 | 1 |
| PbCo0.25Mn0.25Nb0.5O3 | 0 |  | SrZrO3 | 1 |
| PbMg0.25Mn0.25Nb0.5O3 | 0 |  | BaSnO3 | 1 |
| PbZn0.25Mn0.25Nb0.5O3 | 0 |  | BaSb0.5In0.5O3 | 1 |
| PbMg0.25Mn0.25Ta0.5O3 | 0 |  | BaBiO3 | 1 |
| PbNa0.25Sc0.25W0.5O3 | 0 |  | BaW0.5Ba0.5O3 | 1 |
| PbNa0.25Dy0.25W0.5O3 | 0 |  | BaNi0.5W0.5O3 | 1 |
| PbFe0.5Mn0.25W0.25O3 | 0 |  | BaZrO3 | 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 |
| BaW0.5Cu0.5O3 | 0 |  | PbNi0.25Mn0.25Ta0.5O3 | 0 |
| SrW0.5Cu0.5O3 | 0 |  | PbLi0.25Ni0.25W0.5O3 | 0 |
| BaCu0.33Ta0.67O3 | 0 |  | Sr0.5La0.5Cu0.5Nb0.5O3 | 0 |
| PbSc0.67W0.33O3 | 0 |  | SrCo0.5Re0.5O3 | 0 |
| BaBi0.67W0.33O3 | 0 |  | PbMn0.67W0.33O3 | 1 |
| TlMg0.25W0.75O3 | 0 |  | PbZrO3 | 1 |
| PbFe0.5Nb0.5O3 | 0 |  | PbLu0.5Ta0.5O3 | 1 |
| PbFe0.5Nb0.5O3 | 0 |  | PbGa0.5Nb0.5O3 | 1 |
| TlZr0.5W0.5O3 | 0 |  | PbCd0.33Mn0.33W0.34O3 | 1 |
| CdCr0.5Nb0.5O3 | 0 |  | BaZn0.33Nb0.67O3 | 1 |
| PbLi0.25Co0.25W0.5O3 | 0 |  | LaMg0.5Ti0.5O3 | 1 |
| PbLi0.25Y0.25W0.5O3 | 0 |  | CaMnO3 | 1 |
| PbLi0.25Pr0.25W0.5O3 | 0 |  | K0.5Bi0.5ZrO3 | 1 |
| PbLi0.33Zr0.17W0.5O3 | 0 |  | SrMnO3 | 1 |
| PbSc0.56Nb0.11W0.33O3 | 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*/ m2g-1 |  | 化学式 | *SSA*/ m2g-1 | |
| --- | --- | --- | --- | --- | --- |
| La0.9Mg0.1MnO3 | 37.1 |  | PrMn0.8Ni0.2O3 | | 13.97 |
| LaMn0.9Mg0.1O3 | 24.8 |  | PrMn0.6Ni0.4O3 | | 26.61 |
| LaFe0.975Pd0.025O3 | 22 |  | PrMn0.4Ni0.6O3 | | 12.63 |
| LaFe0.95Pd0.05O3 | 27 |  | PrMn0.2Ni0.8O3 | | 8.93 |
| LaCo0.1Mn0.9O3 | 57 |  | LaNi0.4Fe0.6O3 | | 5.4 |
| LaCo0.2Mn0.8O3 | 56 |  | La0.9Ce0.1Ni0.4Fe0.6O3 | | 13.4 |
| LaCo0.8Mn0.2O3 | 31 |  | La0.8Ce0.2Ni0.4Fe0.6O3 | | 21.7 |
| La0.9Zn0.1MnO3 | 28.3 |  | LaMn0.3Cu0.7O3 | | 34 |
| La0.8Zn0.2MnO3 | 26.4 |  | LaMn0.3Fe0.7O3 | | 31 |
| La0.7Zn0.3MnO3 | 20.6 |  | La0.8Sr0.2Mn0.3Cu0.7O3 | | 26 |
| La0.6Zn0.4MnO3 | 13 |  | La0.8Ce0.2Mn0.3Cu0.7O3 | | 25 |
| La0.5Zn0.5MnO3 | 9.2 |  | La0.8Sr0.2Mn0.3Fe0.7O3 | | 24 |
| La0.4Zn0.6MnO3 | 7.7 |  | La0.8Ce0.2Mn0.3Fe0.7O3 | | 27 |
| La0.78K0.02Sr0.2MnO3 | 8.4 |  | LaMn0.9Cu0.1O3 | | 36 |
| La0.74K0.06Sr0.2MnO3 | 5.3 |  | LaMn0.5Cu0.5O3 | | 34 |
| La0.7K0.1Sr0.2MnO3 | 5.7 |  | LaMn0.9Fe0.1O3 | | 33 |
| La0.66K0.14Sr0.2MnO3 | 6.3 |  | LaMn0.5Fe0.5O3 | | 27 |
| La0.62K0.18Sr0.2MnO3 | 10.2 |  | La0.4Sr0.6MnO3 | | 83.7 |
| La0.6K0.2Sr0.2MnO3 | 8.7 |  | La0.2Sr0.8MnO3 | | 114.3 |
| LaNi0.95Ti0.05O3 | 4.527 |  | Al0.05La0.95MnO3 | | 27.7 |
| LaNi0.9Ti0.1O3 | 2.516 |  | Al0.1La0.9MnO3 | | 39.7 |
| LaNi0.85Ti0.15O3 | 3.891 |  | Al0.15La0.85MnO3 | | 42.5 |
| LaNi0.8Ti0.2O3 | 4.584 |  | Al0.2La0.8MnO3 | | 47.3 |
| LaCu0.2Fe0.8O3 | 7.85 |  | Al0.3La0.7MnO3 | | 38.5 |
| LaAl0.2Fe0.8O3 | 6.42 |  | LaCu0.7Zn0.3O3 | | 0.7 |
| LaCo0.75Mn0.25O3 | 8 |  | La0.8Y0.2Cu0.7Zn0.3O3 | | 1.3 |
| LaCo0.75Ni0.25O3 | 10 |  | La0.8Mg0.2Cu0.7Zn0.3O3 | | 1.2 |
| LaCo0.5Ni0.5O3 | 8 |  | La0.8Ce0.2Cu0.7Zn0.3O3 | | 2.3 |
| LaCo0.25Ni0.75O3 | 12 |  | La0.8Zr0.2Cu0.7Zn0.3O3 | | 0.7 |
| LaNi0.25Fe0.75O3 | 7 |  | La0.6Pb0.2Mg0.2MnO3 | | 8.6 |
| LaNi0.5Fe0.5O3 | 6 |  | LaFe0.75Mn0.25O3 | | 25.9 |
| LaNi0.75Fe0.25O3 | 7 |  | LaFe0.5Mn0.5O3 | | 25.2 |
| LaCrO3 | 8.1 |  | LaFe0.25Mn0.75O3 | | 28.2 |
| La0.8Ce0.2Mn0.9Co0.1O3 | 13.8 |  | La0.9Sr0.1MnO3 | | 31.2 |
| La0.8Ce0.2Mn0.7Co0.3O3 | 4.503 |  | La0.9Sm0.1NiO3 | | 5.4 |
| La0.8Ce0.2Mn0.5Co0.5O3 | 9.219 |  | La0.5Sm0.5NiO3 | | 3.4 |
| La0.8Ce0.2Mn0.3Co0.7O3 | 5.712 |  | La0.1Sm0.9NiO3 | | 8.4 |
| La0.8Ca0.2MnO3 | 20.5 |  | Pb0.8Ba0.2TiO3 | | 6.228 |
| La0.67Ca0.33MnO3 | 10.7 |  | Pb0.6Ba0.4TiO3 | | 6.514 |
| La0.5Ca0.5MnO3 | 23 |  | Pb0.5Ba0.5TiO3 | | 10.484 |
| La0.25Ca0.75MnO3 | 20.8 |  | Pb0.4Ba0.6TiO3 | | 13.708 |
| CaMnO3 | 7.1 |  | Pb0.2Ba0.8TiO3 | | 16.592 |
| La0.9Ce0.1Ni0.9Zr0.1O3 | 3 |  | La0.8Ce0.2Mn0.6Cu0.4O3 | | 12.3 |
| La0.9Ce0.1Ni0.8Zr0.2O3 | 5 |  | La0.8Ce0.2Mn0.7Cu0.3O3 | | 22.2 |
| PrMn0.8Fe0.2O3 | 8.34 |  | La0.8Ce0.2Mn0.8Cu0.2O3 | | 12.8 |
| PrMn0.6Fe0.4O3 | 11.67 |  | La0.8Sr0.2Mn0.6Cu0.4O3 | | 28 |
| PrMn0.4Fe0.6O3 | 14.25 |  | La0.8Ce0.1Sr0.1Mn0.6Cu0.4O3 | | 12.4 |
| PrMn0.2Fe0.8O3 | 8.05 |  |  | |  |

表S9 *Eg*回归模型训练数据集

Table S9 Training data of the *Eg* regression model

| 化学式 | *Eg*/eV |  | 化学式 | *Eg*/eV |
| --- | --- | --- | --- | --- |
| PrCuO3 | 3.256 |  | Bi0.9Gd0.1Fe0.9Cr0.1O3 | 2.6 |
| PrCu0.9Zn0.1O3 | 3.088 |  | Pb0.8Co0.15La0.05TiO3 | 3.02 |
| PrCu0.8Zn0.2O3 | 2.933 |  | Pb0.8Co0.1La0.1TiO3 | 3.01 |
| PrCu0.7Zn0.3O3 | 2.898 |  | Pb0.8Co0.05La0.15TiO3 | 2.32 |
| DyCr0.9Co0.1O3 | 2.86 |  | Pb0.8La0.2TiO3 | 3.2 |
| DyCr0.8Co0.2O3 | 2.2 |  | Bi0.99Ba0.01FeO3 | 2.38 |
| DyCr0.7Co0.3O3 | 2.17 |  | Bi0.98Ba0.02FeO3 | 2.36 |
| LaFe0.75Cr0.25O3 | 1.86 |  | Bi0.97Ba0.03FeO3 | 2.21 |
| LaFe0.5Cr0.5O3 | 1.82 |  | Bi0.96Ba0.04FeO3 | 2.04 |
| LaFe0.25Cr0.75O3 | 1.92 |  | Bi0.95Ba0.05FeO3 | 1.97 |
| Bi0.85Gd0.15FeO3 | 1.6 |  | La0.95Na0.05FeO3 | 3.07 |
| La0.95Ba0.05FeO3 | 2.29 |  | La0.9Na0.1FeO3 | 2.81 |
| La0.9Ba0.1FeO3 | 2.4 |  | La0.85Na0.15FeO3 | 2.97 |
| La0.8Ba0.2FeO3 | 2.16 |  | BaZr0.05Ti0.95O3 | 3.36 |
| La0.95Ca0.05FeO3 | 2.34 |  | BaZr0.1Ti0.9O3 | 3.68 |
| La0.9Ca0.1FeO3 | 2.35 |  | BaZr0.15Ti0.85O3 | 3.71 |
| La0.8Ca0.2FeO3 | 2.36 |  | BaZr0.2Ti0.8O3 | 3.57 |
| La0.7Ca0.3FeO3 | 2.27 |  | Bi0.9Ho0.1Fe0.95Mn0.05O3 | 1.79 |
| La0.6Ca0.4FeO3 | 2.26 |  | Bi0.9Ho0.1Fe0.95Co0.05O3 | 1.7 |
| La0.95Sr0.05FeO3 | 2.25 |  | Bi0.9Ho0.1Fe0.95Cu0.05O3 | 2.03 |
| La0.9Sr0.1FeO3 | 2.35 |  | Bi0.9Ho0.1Fe0.95Zn0.05O3 | 1.96 |
| La0.8Sr0.2FeO3 | 2.19 |  | Bi0.9Ho0.1Fe0.95Ni0.05O3 | 1.89 |
| La0.95Mg0.05FeO3 | 2.17 |  | Bi0.9Ho0.1Fe0.95Cr0.05O3 | 1.94 |
| La0.9Mg0.1FeO3 | 2.25 |  | LaMn0.2Fe0.8O3 | 2.49 |
| La0.8Mg0.2FeO3 | 2.29 |  | LaMn0.2Cr0.2Fe0.6O3 | 2.51 |
| La0.7Mg0.3FeO3 | 2.51 |  | LaMn0.2Co0.2Fe0.6O3 | 2.32 |
| La0.6Mg0.4FeO3 | 2.34 |  | LaMn0.2Ni0.2Fe0.6O3 | 2.3 |
| Bi0.75La0.25FeO3 | 1.85 |  | LaMn0.2Cu0.2Fe0.6O3 | 2.29 |
| LaFe0.6Co0.4O3 | 2.39 |  | LaMn0.2Zn0.2Fe0.6O3 | 2.19 |
| LaFe0.5Co0.5O3 | 2.31 |  | LaMnO3 | 2.67 |
| LaFe0.4Co0.6O3 | 2.37 |  | Gd0.9Dy0.1CrO3 | 3.11 |
| Ba0.99Li0.005La0.005TiO3 | 3.02 |  | Gd0.5Dy0.5CrO3 | 3.06 |
| Ba0.98Li0.01La0.01TiO3 | 2.95 |  | Gd0.3Dy0.7CrO3 | 3.03 |
| Ba0.97Li0.015La0.015TiO3 | 2.84 |  | Gd0.1Dy0.9CrO3 | 2.99 |
| Ba0.96Li0.02La0.02TiO3 | 2.77 |  | BiMnO3 | 1.31 |
| PrCrO3 | 3.24 |  | BiMn0.9Cr0.1O3 | 1.32 |
| LaGd0.02Fe0.98O3 | 2.6 |  | BiMn0.9Fe0.1O3 | 1.33 |
| LaGd0.04Fe0.96O3 | 2.58 |  | BiMn0.9Co0.1O3 | 1.36 |
| LaGd0.06Fe0.94O3 | 2.53 |  | BiMn0.9Zn0.1O3 | 1.37 |
| LaGd0.08Fe0.92O3 | 2.52 |  | HoCrO3 | 3.45 |
| LaGd0.1Fe0.9O3 | 2.46 |  | HoCr0.7Fe0.3O3 | 3.39 |
| LaDy0.02Fe0.98O3 | 2.59 |  | BaZrO3 | 3.6553 |
| LaDy0.04Fe0.96O3 | 2.58 |  | BaZr0.95Fe0.05O3 | 3.4943 |
| LaDy0.06Fe0.94O3 | 2.57 |  | BaZr0.9Fe0.1O3 | 3.4277 |
| LaDy0.08Fe0.92O3 | 2.52 |  | BaZr0.8Fe0.2O3 | 3.3207 |
| LaDy0.1Fe0.9O3 | 2.5 |  | BaZr0.7Fe0.3O3 | 3.2201 |
| LaNd0.02Fe0.98O3 | 2.6 |  | BaZr0.6Fe0.4O3 | 3.0032 |
| LaNd0.04Fe0.96O3 | 2.59 |  | BaZr0.5Fe0.5O3 | 2.8435 |
| LaNd0.06Fe0.94O3 | 2.54 |  | BaSnO3 | 3.09 |
| LaNd0.08Fe0.92O3 | 2.52 |  | LaCo0.2Fe0.8O3 | 1.78 |
| LaNd0.1Fe0.9O3 | 2.52 |  | LaCo0.4Fe0.6O3 | 1.7 |
| Bi0.95Ca0.05FeO3 | 2.2 |  | LaCo0.6Fe0.4O3 | 1.68 |
| Bi0.95Ca0.05Fe0.95Ni0.05O3 | 2.17 |  | LaCo0.8Fe0.2O3 | 1.8 |
| Bi0.98Ce0.02FeO3 | 2.01 |  | Bi0.05Ca0.95FeO3 | 2.19 |
| Bi0.96Ce0.04FeO3 | 2 |  | Bi0.1Ca0.9FeO3 | 2.23 |
| Bi0.94Ce0.06FeO3 | 1.97 |  | Bi0.15Ca0.85FeO3 | 2.35 |
| La0.95Ce0.05FeO3 | 2.8 |  | Bi0.2Ca0.8FeO3 | 2.36 |
| La0.9Ce0.1FeO3 | 2.54 |  | Bi0.95Ca0.05Fe0.95Ti0.05O3 | 1.82 |
| La0.85Ce0.15FeO3 | 1.89 |  | Bi0.9Ca0.1Fe0.9Ti0.1O3 | 1.96 |
| GdMn0.7Ni0.3O3 | 3.2 |  | Bi0.85Ca0.15Fe0.85Ti0.15O3 | 2.08 |
| GdCr0.9Mn0.1O3 | 3.77 |  | Bi0.8Ca0.2Fe0.8Ti0.2O3 | 2.14 |
| GdCr0.8Mn0.2O3 | 3.72 |  | Bi0.75Ca0.25Fe0.75Ti0.25O3 | 2.25 |
| GdCr0.7Mn0.3O3 | 3.69 |  | Bi0.9Y0.1FeO3 | 2.5 |
| GdCr0.6Mn0.4O3 | 3.71 |  | Bi0.9Y0.1Fe0.97Co0.03O3 | 2.42 |
| Bi0.98Ho0.02Fe0.99Cr0.01O3 | 2.22 |  | Bi0.9Y0.1Fe0.95Co0.05O3 | 2.42 |
| Bi0.98Ho0.02Fe0.98Cr0.02O3 | 2.66 |  | Bi0.9Y0.1Fe0.9Co0.1O3 | 2.45 |
| Bi0.98Ho0.02Fe0.97Cr0.03O3 | 2.37 |  | BiFe0.95Co0.05O3 | 1.95 |
| Bi0.98Ho0.02Fe0.96Cr0.04O3 | 2.7 |  | BiFe0.85Co0.15O3 | 1.91 |
| Bi0.98La0.02FeO3 | 1.99 |  | BiFe0.8Co0.2O3 | 1.64 |
| Bi0.98La0.02Fe0.9Se0.1O3 | 1.96 |  | BiFe0.75Co0.25O3 | 1.28 |
| Bi0.98La0.02Fe0.75Se0.25O3 | 1.8 |  | Bi0.95Ho0.05FeO3 | 2.09 |
| Bi0.98La0.02Fe0.5Se0.5O3 | 1.77 |  | Bi0.85Ho0.15FeO3 | 2.03 |
| Bi0.98La0.02SeO3 | 2.05 |  | Bi0.8Ho0.2FeO3 | 2.01 |
| LaNi0.2Fe0.8O3 | 1.63 |  | Bi0.9Nd0.1FeO3 | 2.89 |
| LaNi0.4Fe0.6O3 | 1.56 |  | Bi0.9Nd0.1Fe0.9Co0.1O3 | 2.93 |
| LaNi0.6Fe0.4O3 | 1.65 |  | BiFe0.95Mn0.05O3 | 2.6 |
| LaNi0.8Fe0.2O3 | 1.77 |  | Bi0.97Sm0.03Fe0.95Mn0.05O3 | 2.62 |
| NdFeO3 | 3.35 |  | Bi0.94Sm0.06Fe0.95Mn0.05O3 | 2.65 |
| NdFe0.9Co0.1O3 | 3.26 |  | Bi0.91Sm0.09Fe0.95Mn0.05O3 | 2.67 |
| NdFe0.8Co0.2O3 | 3.2 |  | Bi0.9Gd0.1Fe0.95Mn0.05O3 | 1.76 |
| NdFe0.7Co0.3O3 | 3.09 |  | Bi0.9Gd0.1Fe0.9Mn0.1O3 | 1.62 |
| NdFe0.6Co0.4O3 | 3.04 |  | Bi0.9Gd0.1Fe0.85Mn0.15O3 | 1.68 |
| La0.75Ba0.25FeO3 | 2.98 |  | Bi0.9Gd0.1Fe0.8Mn0.2O3 | 1.52 |
| La0.75Ba0.2Sr0.05FeO3 | 3.09 |  | Bi0.9Gd0.1Fe0.75Mn0.25O3 | 1.47 |
| La0.75Ba0.15Sr0.1FeO3 | 3.2 |  | Bi0.9Ca0.1FeO3 | 2.47 |
| La0.75Ba0.1Sr0.15FeO3 | 3.25 |  | Bi0.8Ca0.2FeO3 | 2.43 |
| BaTi0.75Mn0.25O3 | 2.93 |  | Bi0.7Ca0.3FeO3 | 2.385 |
| BaTi0.5Mn0.5O3 | 2.83 |  | Bi0.6Ca0.4FeO3 | 2.38 |
| BaTi0.25Mn0.75O3 | 2.71 |  | Bi0.5Ca0.5FeO3 | 2.37 |
| YbFeO3 | 1.55 |  | La0.9Sr0.1Fe0.9Ni0.1O3 | 2.28 |
| Bi0.9Gd0.1Fe0.975Cr0.025O3 | 2.56 |  | La0.8Sr0.2Fe0.8Ni0.2O3 | 2.36 |
| Bi0.9Gd0.1Fe0.95Cr0.05O3 | 2.58 |  | Bi0.85Nd0.15FeO3 | 2.8 |
| Bi0.9Gd0.1Fe0.925Cr0.075O3 | 2.59 |  |  |  |

表S10 *Tc*回归模型训练数据集

Table S10 Training data of the *Tc* regression model

| 化学式 | *Tc*/K | 化学式 | *Tc*/K |
| --- | --- | --- | --- |
| La0.67Sr0.33MnO3 | 355 | Pb0.86Gd0.08La0.06Zr0.52Ti0.48O3 | 347 |
| La0.67Sr0.23K0.1MnO3 | 360 | La0.603Pr0.067Pb0.33MnO3 | 353 |
| La0.67Sr0.23Pb0.1MnO3 | 365 | La0.536Pr0.134Pb0.33MnO3 | 346 |
| La0.7Ba0.15Sr0.15CoO3 | 228 | La0.469Pr0.201Pb0.33MnO3 | 330 |
| Ba0.8Sr0.2TiO3 | 351.15 | La0.765Sm0.085K0.15MnO3 | 170 |
| Ba0.7Sr0.3TiO3 | 306.65 | La0.68Sm0.17K0.15MnO3 | 145 |
| Ba0.6Sr0.4TiO3 | 269.65 | La0.595Sm0.255K0.15MnO3 | 130 |
| Ba0.5Sr0.5TiO3 | 231.48 | La0.7Ca0.15Ba0.15MnO3 | 299.2 |
| Ba0.4Sr0.6TiO3 | 189.15 | La0.67Ca0.33MnO3 | 272 |
| La0.8Ba0.05Sr0.15MnO3 | 320 | La0.67Dy0.03Sr0.3MnO3 | 274.94 |
| La0.75K0.05Ba0.05Sr0.15MnO3 | 335 | La0.7Nd0.05Ba0.25MnO3 | 293 |
| La0.7K0.1Ba0.05Sr0.15MnO3 | 345 | La0.7Nd0.1Ba0.2MnO3 | 257 |
| La0.65K0.15Ba0.05Sr0.15MnO3 | 355 | La0.6Gd0.1Sr0.3MnO3 | 350 |
| La0.6K0.2Ba0.05Sr0.15MnO3 | 360 | La0.65Ca0.2Na0.075K0.075MnO3 | 296 |
| La0.6Nd0.1Ca0.3MnO3 | 171 | La0.67Sr0.22Ba0.11MnO3 | 360 |
| La0.6Sm0.1Ca0.3MnO3 | 135 | La0.67Sr0.22Ba0.11Mn0.9Co0.1O3 | 300 |
| La0.6Gd0.1Ca0.3MnO3 | 125 | La0.67Sr0.22Ba0.11Mn0.8Co0.2O3 | 220 |
| La0.6Dy0.1Ca0.3MnO3 | 111 | La0.67Sr0.22Ba0.11Mn0.7Co0.3O3 | 185 |
| La0.6Ca0.2Na0.2MnO3 | 275 | La0.765Pr0.085K0.15MnO3 | 225 |
| La0.7Sr0.3Mn0.9Cu0.1O3 | 320 | La0.595Pr0.255K0.15MnO3 | 183 |
| La0.6Bi0.1Sr0.3Mn0.9Cu0.1O3 | 300 | La0.425Pr0.425K0.15MnO3 | 158 |
| La0.6Bi0.1Sr0.25Ca0.05Mn0.9Cu0.1O3 | 290 | Pr0.8Na0.15K0.05MnO3 | 180 |
| La0.67Ca0.33Mn0.98Ni0.02O3 | 244 | Pr0.8Na0.1K0.1MnO3 | 175 |
| La0.8Na0.2MnO3 | 297 | Pr0.8Na0.05K0.15MnO3 | 160 |
| La0.8Na0.2Mn0.97Ni0.03O3 | 275 | La0.7Ca0.21Ag0.09MnO3 | 263 |
| La0.8Na0.2Mn0.94Ni0.06O3 | 257 | La0.7Ca0.15Sr0.15Mn0.875Ga0.125O3 | 221.4 |
| La0.9Sr0.1MnO3 | 154.8 | La0.7Ca0.15Sr0.15Mn0.85Ga0.15O3 | 208.21 |
| La0.85Sr0.15MnO3 | 235.8 | La0.7Ca0.15Sr0.15Mn0.825Ga0.175O3 | 166.18 |
| La0.8Sr0.2MnO3 | 305.9 | La0.7Ca0.15Sr0.15Mn0.8Ga0.2O3 | 137.7 |
| La0.8Ag0.2MnO3 | 306 | La0.65Sr0.35MnO3 | 362 |
| La0.7Ca0.29K0.01MnO3 | 265.01 | La0.603Sm0.067Pb0.33MnO3 | 341 |
| La0.7Ca0.28K0.02MnO3 | 266.02 | La0.536Sm0.134Pb0.33MnO3 | 311 |
| La0.7Ca0.27K0.03MnO3 | 270.01 | La0.469Sm0.201Pb0.33MnO3 | 286 |
| La0.7Ca0.26K0.04MnO3 | 277.01 | NdMnO3 | 67.2 |
| La0.67Ca0.29Sr0.04MnO3 | 276 | Nd0.85Na0.15MnO3 | 99.1 |
| La0.8Na0.2Mn0.97Bi0.03O3 | 257 | Nd0.85K0.15MnO3 | 98.6 |
| La0.65Ca0.35Mn0.95Ni0.05O3 | 272 | Pr0.6La0.1Mg0.3MnO3 | 64 |
| La0.65Ca0.35Mn0.9Ni0.1O3 | 236 | Pr0.6La0.1Mg0.3Mn0.9Fe0.1O3 | 65 |
| La0.65Ca0.35Mn0.85Ni0.15O3 | 194 | Pr0.6La0.1Mg0.3Mn0.7Fe0.3O3 | 380 |
| Ba0.85Ca0.15Zr0.1Ti0.9O3 | 385.15 | La0.7Sr0.21K0.09MnO3 | 295 |
| BaTiO3 | 403.46 | Pr0.6La0.1Ca0.3MnO3 | 94 |
| Ba0.96Ca0.04TiO3 | 413.28 | Pr0.6La0.1Ca0.3Mn0.9Fe0.1O3 | 65 |
| Ba0.95Ca0.05TiO3 | 416.91 | Pr0.6La0.1Ca0.3Mn0.8Fe0.2O3 | 60 |
| Ba0.9Ca0.1TiO3 | 414.53 | Pr0.6La0.1Ca0.3Mn0.7Fe0.3O3 | 59 |
| La0.595Gd0.005Sr0.4MnO3 | 354.7 | La0.7Sr0.3Mn0.9Fe0.1O3 | 261 |
| La0.5Gd0.1Sr0.4MnO3 | 336.3 | La0.7Pb0.3Mn0.9Fe0.1O3 | 215 |
| La0.5Ba0.5MnO3 | 339 | La0.7Ba0.3Mn0.9Fe0.1O3 | 194 |
| La0.603Pr0.067Ca0.33MnO3 | 233 | Pr0.67Ca0.33FeO3 | 208 |
| La0.536Pr0.134Ca0.33MnO3 | 228 | Pr0.67Ca0.33Fe0.1Mn0.9O3 | 176 |
| La0.469Pr0.201Ca0.33MnO3 | 180 | Pr0.67Ca0.33Fe0.2Mn0.8O3 | 135 |
| La0.402Pr0.268Ca0.33MnO3 | 171 | Pr0.67Ca0.33Fe0.3Mn0.7O3 | 105 |
| Pb0.94La0.06Zr0.52Ti0.48O3 | 350 | La0.65Ca0.35MnO3 | 267.9 |
| Pb0.92Gd0.02La0.06Zr0.52Ti0.48O3 | 373 | La0.67Pb0.28Ag0.05MnO3 | 332 |
| Pb0.9Gd0.04La0.06Zr0.52Ti0.48O3 | 366 | La0.67Pb0.23Ag0.1MnO3 | 311 |
| Pb0.88Gd0.06La0.06Zr0.52Ti0.48O3 | 399 | La0.67Pb0.18Ag0.15MnO3 | 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* |
| MnFeO3 | 0.13 | Na0.47Bi0.47Ba0.06TiO3 | 0.048 |
| Gd0.4Mn0.6Fe0.96Cu0.04O3 | 0.12 | Pb0.94La0.06Zr0.52Ti0.48O3 | 0.03 |
| Gd0.6Mn0.4Fe0.94Cu0.06O3 | 0.1 | Pb0.92Gd0.02La0.06Zr0.52Ti0.48O3 | 0.027 |
| Gd0.8Mn0.2Fe0.92Cu0.08O3 | 0.08 | Pb0.90Gd0.04La0.06Zr0.52Ti0.48O3 | 0.032 |
| Na0.425K0.075Bi0.5TiO3 | 0.051 | Pb0.88Gd0.06La0.06Zr0.52Ti0.48O3 | 0.029 |
| Pb0.5Sr0.5TiO3 | 0.056 | Pb0.86Gd0.08La0.06Zr0.52Ti0.48O3 | 0.028 |
| Pb0.5Sr0.5Ti0.99Fe0.01O3 | 0.045 | Ba0.95Tm0.05TiO3 | 0.0231 |
| Pb0.5Sr0.5Ti0.95Fe0.05O3 | 0.044 | Bi0.9Sm0.1FeO3 | 0.08 |
| Pb0.5Sr0.5Ti0.9Fe0.1O3 | 0.016 | BiFeO3 | 0.065 |
| Ba0.95La0.05TiO3 | 0.005 | BiFe0.97Ti0.03O3 | 0.061 |
| Pb0.9Na0.05Sm0.05TiO3 | 0.012 | Na0.5K0.5NbO3 | 0.05 |
| Pb0.8Na0.1Sm0.1TiO3 | 0.017 | Ba0.7Sr0.3Zr0.01Ti0.99O3 | 0.06 |
| Pb0.7Na0.15Sm0.15TiO3 | 0.026 | Ba0.7Sr0.3Zr0.02Ti0.98O3 | 0.05 |
| Pb0.6Na0.2Sm0.2TiO3 | 0.038 | Ba0.7Sr0.3Zr0.03Ti0.97O3 | 0.02 |
| Pb0.5Na0.25Sm0.25TiO3 | 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*/ m2g-1 | | Exp. *SSA*/ m2g-1 |
| --- | --- | --- | --- |
| LaMnO3 | | 31.854 | 30.8 |
| LaCo0.5Mn0.5O3 | | 19.938 | 7 |
| LaCoO3 | | 5.401 | 5 |
| La0.8Sr0.2MnO3 | | 19.049 | 8.3 |
| LaTi0.2Fe0.8O3 | | 27.675 | 12.95 |
| LaNiO3 | | 7.506 | 8 |
| LaFeO3 | | 14.869 | 10 |
| LaMn0.7Cu0.3O3 | | 30.441 | 29 |
| LaMn0.7Fe0.3O3 | | 31.199 | 31 |
| La0.8Ce0.2MnO3 | | 18.215 | 10.727 |

表S13 *Eg*模型测试集模型预报值与实验值

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

|  |  |  |
| --- | --- | --- |
| 化学式 | Pred. *Eg*/eV | Exp. *Eg*/eV |
| BiFeO3 | 2.188 | 2.18 |
| BiFe0.9Co0.1O3 | 2.163 | 1.81 |
| DyCrO3 | 2.902 | 2.96 |
| LaFeO3 | 2.373 | 2.52 |
| LaCrO3 | 2.433 | 2.34 |
| GdCrO3 | 3.443 | 3.36 |
| LaNiO3 | 1.572 | 1.8 |
| BaTiO3 | 3.019 | 3.13 |
| Bi0.9Gd0.1FeO3 | 2.101 | 2.07 |

表S14 *Tc*模型测试集模型预报值与实验值

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

|  |  |  |
| --- | --- | --- |
| 化学式 | Pred. *Tc*/K | Exp. *Tc*/K |
| La0.7Ca0.3MnO3 | 237.942 | 215 |
| La0.67Pb0.33MnO3 | 340.995 | 349 |
| La0.75Sr0.25MnO3 | 323.147 | 344.9 |
| La0.6Sr0.4MnO3 | 371.224 | 366.53 |
| La0.85K0.15MnO3 | 227.954 | 238 |
| La0.7Sr0.3MnO3 | 347.070 | 361.5 |
| La0.7Ba0.3MnO3 | 311.931 | 303 |
| La0.7Ca0.15Sr0.15MnO3 | 296.484 | 319.2 |

表S15 *tanδ*模型测试集模型预报值与实验值

Table S15: Predicted and experimental *tanδ* with the lowest error of the testing set

|  |  |  |
| --- | --- | --- |
| 化学式 | Pred. *tanδ* | Exp. *tanδ* |
| Bi0.5Na0.5TiO3 | 0.052 | 0.07 |
| BaTiO3 | 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*/ m2g-1 | Exp. *SSA*/ m2g-1 |
| CaFeO3 | 13.951 | 17.37 |
| Ca0.5Pr0.5FeO3 | 24.595 | 66.65 |
| La0.6Sr0.4MnO3 | 33.944 | 96.4 |

表S17 *Eg*模型可疑样本模型预报值与实验值

Table S17: Predicted and experimental *Eg* of the suspected samples

|  |  |  |
| --- | --- | --- |
| 化学式 | Pred. *Eg*/eV | Exp. *Eg*/eV |
| LaNi0.8Co0.2O3 | 1.598 | 3.825 |
| LaNi0.6Co0.4O3 | 1.642 | 3.826 |
| LaNi0.4Co0.6O3 | 1.703 | 3.82 |
| CoFeO3 | 3.268 | 1.84 |

表S18 *Tc*模型可疑样本模型预报值与实验值

Table S18: Predicted and experimental *Tc* of the suspected samples

|  |  |  |
| --- | --- | --- |
| 化学式 | Pred. *Tc*/K | Exp. *Tc*/K |
| Pr0.6La0.1Mg0.3Mn0.8Fe0.2O3 | 266.598 | 957 |

表S19 *tanδ*模型可疑样本模型预报值与实验值

Table S19: Predicted and experimental *tanδ* of the suspected samples

|  |  |  |
| --- | --- | --- |
| 化学式 | Pred. *tanδ* | Exp. *tanδ* |
| Gd0.2Mn0.8Fe0.98Cu0.02O3 | 0.119 | 0.2 |
| GdFe0.9Cu0.1O3 | 0.077 | 0.129 |
| Na0.5Ba0.5Ti0.99W0.01O3 | 0.053 | 0.094 |
| SrTiO3 | 0.053 | 0.45 |
| Bi0.5K0.5TiO3 | 0.035 | 0.0584 |
| BaTi0.98Ni0.02O3 | 0.032 | 0.27 |
| BaTi0.96Ni0.04O3 | 0.033 | 0.16 |
| BaTi0.94Ni0.06O3 | 0.034 | 0.11 |
| Ba0.7Sr0.3TiO3 | 0.039 | 0.27 |

表S20 ABO3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 ABO3 type perovskites and corresponding oxide ionic conductivity of the data set collected form publications

| 化学式 | *lnσ* |  | 化学式 | *lnσ* |
| --- | --- | --- | --- | --- |
| BaZrO3-δ | -14 |  | La0.5Sr0.5Ga0.65Zr0.35O3-δ | -4.93 |
| PrGaO3-δ | -12.37 |  | PrGa0.85Mg0.15O3-δ | -4.81 |
| SrSc0.5Al0.5O3-δ | -10.87 |  | Nd0.9Ca0.1Ga0.9Mg0.1O3-δ | -4.79 |
| Yb0.9Ca0.1AlO3-δ | -10.82 |  | La0.9Sr0.1InO3-δ | -4.67 |
| SrSc0.4Y0.1Al0.5O3-δ | -10.27 |  | La0.5Sr0.5Ga0.7Zr0.3O3-δ | -4.61 |
| SrSc0.45Y0.05Al0.5O3-δ | -10.11 |  | La0.9Sr0.1Ga0.9Al0.1O3-δ | -4.44 |
| Nd0.9Ba0.1AlO3-δ | -9.42 |  | La0.9Sr0.1ScO3-δ | -4.37 |
| Sr0.8Ba0.2Sc0.5Al0.5O3-δ | -8.98 |  | Pr0.9Ca0.1AlO3-δ | -4.14 |
| SrSc0.5Al0.45Zn0.05O3-δ | -8.84 |  | CaTi0.95Sc0.05O3-δ | -4.14 |
| SrSc0.5Al0.45Mg0.05O3-δ | -8.73 |  | CaTi0.85Sc0.15O3-δ | -4.07 |
| SrSc0.5Al0.35Mg0.15O3-δ | -8.73 |  | La0.9Sr0.1Sc0.9Mg0.1O3-δ | -3.96 |
| Nd0.9Ca0.1Al0.9Zn0.1O3-δ | -8.57 |  | CaTi0.75Sc0.25O3-δ | -3.91 |
| SrSc0.5Al0.4Zn0.1O3-δ | -8.57 |  | LaSc0.9Mg0.1O3-δ | -3.91 |
| La0.5Sr0.5Ga0.55Zr0.45O3-δ | -8.54 |  | Sm0.85Ca0.15AlO3-δ | -3.86 |
| CaTiO3-δ | -8.52 |  | Nd0.9Ca0.1Ga0.95Mg0.05O3-δ | -3.85 |
| Nd0.9Ba0.1GaO3-δ | -8.36 |  | La0.9Sr0.1Ga0.9In0.1O3-δ | -3.85 |
| Nd0.9Ca0.1Al0.9Mg0.1O3-δ | -8.11 |  | CaTi0.9Sc0.1O3-δ | -3.82 |
| BaZr0.8In0.2O3-δ | -8.04 |  | Sm0.78Ca0.22AlO3-δ | -3.77 |
| SrSc0.5Al0.4Mg0.1O3-δ | -7.94 |  | La0.72Yb0.08Sr0.2Ga0.8Mg0.2O3-δ | -3.64 |
| Nd0.9Ca0.1Al0.9Zr0.1O3-δ | -7.92 |  | PrGa0.95Mg0.05O3-δ | -3.62 |
| Nd0.9Sr0.1AlO3-δ | -7.71 |  | NdGa0.9Mg0.1O3-δ | -3.49 |
| La0.7Ca0.3AlO3-δ | -7.58 |  | Sm0.82Ca0.18AlO3-δ | -3.47 |
| Nd0.9Ca0.1Al0.9Be0.1O3-δ | -7.44 |  | Sm0.8Ca0.2AlO3-δ | -3.35 |
| La0.9Ca0.1AlO3-δ | -7.32 |  | PrGa0.75Mg0.25O3-δ | -3.27 |
| CaTi0.75Ga0.25O3-δ | -7.29 |  | La0.72Y0.08Sr0.2Ga0.8Mg0.2O3-δ | -3.13 |
| SrTiO3-δ | -7.25 |  | La0.75Sr0.25Ga0.9Mg0.1O3-δ | -3.11 |
| BaZr0.7In0.3O3-δ | -7.21 |  | PrGa0.9Mg0.1O3-δ | -2.99 |
| BaZr0.6In0.4O3-δ | -7.14 |  | La0.72Cd0.08Sr0.2Ga0.8Mg0.2O3-δ | -2.97 |
| Sr0.9Ba0.1Sc0.6Al0.3Mg0.1O3-δ | -6.86 |  | Pr0.93Ca0.07Ga0.85Mg0.15O3-δ | -2.9 |
| La0.9Ba0.1AlO3-δ | -6.86 |  | Pr0.93Sr0.07Ga0.85Mg0.15O3-δ | -2.67 |
| Nd0.9Ca0.1AlO3-δ | -6.75 |  | La0.72Sm0.08Sr0.2Ga0.8Mg0.2O3-δ | -2.56 |
| Y0.9Ca0.1AlO3-δ | -6.68 |  | La0.85Sr0.15Ga0.95Mg0.05O3-δ | -2.51 |
| La0.5Sr0.5Ga0.6Zr0.4O3-δ | -6.56 |  | La0.9Sr0.1Ga0.95Mg0.05O3-δ | -2.42 |
| Nd0.9Ca0.1Al0.9Ga0.1O3-δ | -6.52 |  | La0.8Sr0.2Ga0.95Mg0.05O3-δ | -2.39 |
| BaIn0.8Zr0.2O3-δ | -6.31 |  | La0.9Sr0.1Ga0.9Mg0.1O3-δ | -2.36 |
| La0.9Ca0.1GaO3-δ | -6.31 |  | La0.75Sr0.25Ga0.85Mg0.15O3-δ | -2.26 |
| Nd0.9Sr0.1GaO3-δ | -6.29 |  | La0.9Sr0.1Ga0.85Mg0.15O3-δ | -2.15 |
| La0.9Sr0.1In0.9Mg0.1O3-δ | -6.21 |  | La0.85Sr0.15Ga0.9Mg0.1O3-δ | -2.11 |
| BaIn0.7Zr0.3O3-δ | -6.17 |  | La0.8Sr0.2Ga0.85Mg0.15O3-δ | -2.1 |
| La0.9Sr0.1AlO3-δ | -6.01 |  | La0.85Sr0.15Ga0.8Mg0.2O3-δ | -2.09 |
| Gd0.9Ca0.1AlO3-δ | -5.99 |  | La0.9Sr0.1Ga0.75Mg0.25O3-δ | -2.07 |
| CaTi0.8Ga0.2O3-δ | -5.95 |  | La0.8Sr0.2Ga0.9Mg0.1O3-δ | -2.06 |
| La0.9Sr0.1LuO3-δ | -5.89 |  | La0.85Sr0.15Ga0.85Mg0.15O3-δ | -2.03 |
| La0.9Ba0.1GaO3-δ | -5.89 |  | La0.8Sr0.2Ga0.8Mg0.2O3-δ | -2.03 |
| CaTi0.5Al0.5O3-δ | -5.81 |  | La0.8Sr0.2Ga0.8Mg0.19Co0.01O3-δ | -1.93 |
| BaIn0.6Zr0.4O3-δ | -5.64 |  | La0.8Sr0.2Ga0.8Mg0.15Co0.05O3-δ | -1.71 |
| BaIn0.9Zr0.1O3-δ | -5.64 |  | La0.8Sr0.2Ga0.8Mg0.13Co0.07O3-δ | -1.7 |
| CaTi0.9Ga0.1O3-δ | -5.6 |  | La0.8Sr0.2Ga0.8Mg0.115Co0.085O3-δ | -1.57 |
| Nd0.9Ca0.1GaO3-δ | -5.48 |  | La0.8Sr0.2Ga0.8Mg0.17Ni0.03O3-δ | -1.52 |
| CaTi0.85Ga0.15O3-δ | -5.47 |  | La0.8Sr0.2Ga0.8Mg0.11Co0.09O3-δ | -1.45 |
| CaTi0.95Mg0.05O3-δ | -5.3 |  | La0.8Sr0.2Ga0.8Mg0.15Ni0.05O3-δ | -1.45 |
| CaTi0.9Al0.1O3-δ | -5.12 |  | La0.8Sr0.2Ga0.8Mg0.13Ni0.07O3-δ | -1.43 |
| Sm0.9Ca0.1AlO3-δ | -5.07 |  | La0.8Sr0.2Ga0.8Mg0.1Ni0.1O3-δ | -1.31 |
| La0.9Sr0.1Al0.9Mg0.1O3-δ | -4.96 |  | La0.8Sr0.2Ga0.8Mg0.05Co0.15O3-δ | -1.24 |
| BaIn0.5Zr0.5O3-δ | -4.95 |  | La0.7Sr0.3Ga0.7Fe0.2Mg0.1O3-δ | -1.24 |
| Nd0.9Ca0.1Al0.5Ga0.5O3-δ | -4.93 |  | La0.8Sr0.2Ga0.8Ni0.2O3-δ | 0.04 |
| La0.5Sr0.5Ga0.75Zr0.25O3-δ | -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* |
| --- | --- | --- | --- | --- |
| Pr0.7Ba0.3Ga0.87Al0.13O3-δ | -1.385 |  | La0.8Sr0.2Ga0.801Al0.199O3-δ | -1.313 |
| Pr0.78Ba0.22Ga0.805Ti0.195O3-δ | -1.423 |  | La0.8Sr0.2Ga0.798Ti0.202O3-δ | -1.430 |
| Pr0.77Ba0.23Ga0.805Ti0.195O3-δ | -1.413 |  | La0.8Sr0.2Ga0.796Ti0.204O3-δ | -1.423 |
| Pr0.765Ba0.235Ga0.808Ti0.192O3-δ | -1.409 |  | La0.8Sr0.2Ga0.795Al0.205O3-δ | -1.426 |
| Pr0.72Ba0.28Ga0.836Ti0.164O3-δ | -1.412 |  | La0.8Sr0.2Ga0.793Ti0.207O3-δ | -1.447 |
| Pr0.72Ba0.28Ga0.865Al0.135O3-δ | -1.434 |  | La0.8Sr0.2Ga0.788Ti0.212O3-δ | -1.395 |
| Pr0.72Ba0.28Ga0.855Ti0.145O3-δ | -1.450 |  | La0.8Sr0.2Ga0.781Ti0.219O3-δ | -1.355 |
| Pr0.72Ba0.28Ga0.844Ti0.156O3-δ | -1.407 |  | La0.8Sr0.2Ga0.77Ti0.23O3-δ | -1.398 |
| Pr0.72Ba0.28Ga0.841Al0.159O3-δ | -1.429 |  | La0.8Sr0.2Ga0.775Ti0.225O3-δ | -1.344 |
| Pr0.72Ba0.28Ga0.833Ti0.167O3-δ | -1.420 |  | La0.8Sr0.2Ga0.81Al0.19O3-δ | -1.327 |
| Pr0.72Ba0.28Ga0.829Ti0.171O3-δ | -1.382 |  | La0.8Sr0.2Ga0.816Al0.184O3-δ | -1.433 |
| Pr0.72Ba0.28Ga0.828Ti0.172O3-δ | -1.436 |  | La0.81Sr0.19Ga0.808Al0.192O3-δ | -1.444 |
| Pr0.72Ba0.28Ga0.795Sc0.205O3-δ | -1.413 |  | La0.811Sr0.189Ga0.801Al0.199O3-δ | -1.430 |
| Pr0.72Ba0.28Ga0.792Sc0.208O3-δ | -1.411 |  | La0.806Sr0.194Ga0.811Al0.189O3-δ | -1.421 |
| Pr0.72Ba0.28Ga0.785Sc0.215O3-δ | -1.414 |  | La0.805Sr0.195Ga0.818Al0.182O3-δ | -1.448 |
| Pr0.72Ba0.28Ga0.845Al0.155O3-δ | -1.429 |  | La0.805Sr0.195Ga0.806Ti0.194O3-δ | -1.405 |
| Pr0.71Ba0.29Ga0.8Sc0.2O3-δ | -1.435 |  | La0.805Sr0.195Ga0.792Ti0.208O3-δ | -1.448 |
| Pr0.71Ba0.29Ga0.871Al0.129O3-δ | -1.376 |  | La0.805Sr0.195Ga0.78Ti0.22O3-δ | -1.350 |
| Pr0.71Ba0.29Ga0.86Ti0.14O3-δ | -1.443 |  | La0.805Sr0.195Ga0.786Ti0.214O3-δ | -1.397 |
| Pr0.71Ba0.29Ga0.866Al0.134O3-δ | -1.395 |  | La0.805Sr0.195Ga0.773Ti0.227O3-δ | -1.400 |
| Pr0.71Ba0.29Ga0.865Ti0.135O3-δ | -1.443 |  | La0.804Sr0.196Ga0.816Al0.184O3-δ | -1.433 |
| Pr0.71Ba0.29Ga0.862Ti0.138O3-δ | -1.436 |  | La0.804Sr0.196Ga0.805Ti0.195O3-δ | -1.403 |
| Pr0.71Ba0.29Ga0.861Ti0.139O3-δ | -1.432 |  | La0.803Sr0.197Ga0.8Al0.2O3-δ | -1.387 |
| Pr0.71Ba0.29Ga0.861Al0.139O3-δ | -1.397 |  | La0.803Sr0.197Ga0.774Ti0.226O3-δ | -1.343 |
| Pr0.71Ba0.29Ga0.85Ti0.15O3-δ | -1.415 |  | La0.802Sr0.198Ga0.802Ti0.198O3-δ | -1.425 |
| Pr0.71Ba0.29Ga0.859Ti0.141O3-δ | -1.372 |  | La0.801Sr0.199Ga0.819Al0.181O3-δ | -1.445 |
| Pr0.71Ba0.29Ga0.857Ti0.143O3-δ | -1.426 |  | La0.801Sr0.199Ga0.797Ti0.203O3-δ | -1.421 |
| Pr0.71Ba0.29Ga0.852Al0.148O3-δ | -1.443 |  | La0.79Sr0.21Ga0.814Al0.186O3-δ | -1.437 |
| Pr0.71Ba0.29Ga0.84Ti0.16O3-δ | -1.416 |  | La0.79Sr0.21Ga0.806Ti0.194O3-δ | -1.438 |
| Pr0.71Ba0.29Ga0.841Ti0.159O3-δ | -1.417 |  | La0.79Sr0.21Ga0.801Al0.199O3-δ | -1.399 |
| Pr0.71Ba0.29Ga0.837Ti0.163O3-δ | -1.420 |  | La0.79Sr0.21Ga0.78Ti0.22O3-δ | -1.415 |
| Pr0.71Ba0.29Ga0.831Ti0.169O3-δ | -1.437 |  | La0.79Sr0.21Ga0.782Ti0.218O3-δ | -1.415 |
| Pr0.71Ba0.29Ga0.82Sc0.18O3-δ | -1.424 |  | La0.799Sr0.201Ga0.81Ti0.19O3-δ | -1.446 |
| Pr0.71Ba0.29Ga0.829Ti0.171O3-δ | -1.444 |  | La0.799Sr0.201Ga0.789Ti0.211O3-δ | -1.397 |
| Pr0.71Ba0.29Ga0.823Sc0.177O3-δ | -1.430 |  | La0.799Sr0.201Ga0.781Ti0.219O3-δ | -1.357 |
| Pr0.71Ba0.29Ga0.79Sc0.21O3-δ | -1.414 |  | La0.799Sr0.201Ga0.779Ti0.221O3-δ | -1.348 |
| Pr0.71Ba0.29Ga0.795Sc0.205O3-δ | -1.414 |  | La0.799Sr0.201Ga0.774Ti0.226O3-δ | -1.397 |
| Pr0.71Ba0.29Ga0.785Sc0.215O3-δ | -1.415 |  | La0.798Sr0.202Ga0.812Al0.188O3-δ | -1.368 |
| Pr0.719Ba0.281Ga0.871Al0.129O3-δ | -1.433 |  | La0.798Sr0.202Ga0.807Ti0.193O3-δ | -1.405 |
| Pr0.719Ba0.281Ga0.869Al0.131O3-δ | -1.405 |  | La0.798Sr0.202Ga0.805Ti0.195O3-δ | -1.410 |
| Pr0.719Ba0.281Ga0.832Ti0.168O3-δ | -1.375 |  | La0.798Sr0.202Ga0.79Ti0.21O3-δ | -1.412 |
| Pr0.718Ba0.282Ga0.869Al0.131O3-δ | -1.361 |  | La0.798Sr0.202Ga0.795Ti0.205O3-δ | -1.425 |
| Pr0.718Ba0.282Ga0.856Al0.144O3-δ | -1.435 |  | La0.797Sr0.203Ga0.809Al0.191O3-δ | -1.393 |
| Pr0.716Ba0.284Ga0.86Ti0.14O3-δ | -1.422 |  | La0.797Sr0.203Ga0.802Al0.198O3-δ | -1.379 |
| Pr0.716Ba0.284Ga0.861Ti0.139O3-δ | -1.431 |  | La0.796Sr0.204Ga0.808Ti0.192O3-δ | -1.444 |
| Pr0.716Ba0.284Ga0.849Al0.151O3-δ | -1.386 |  | La0.795Sr0.205Ga0.807Ti0.193O3-δ | -1.448 |
| Pr0.716Ba0.284Ga0.798Sc0.202O3-δ | -1.418 |  | La0.795Sr0.205Ga0.779Ti0.221O3-δ | -1.413 |
| Pr0.715Ba0.285Ga0.86Al0.14O3-δ | -1.417 |  | La0.78Sr0.22Ga0.81Al0.19O3-δ | -1.413 |
| Pr0.715Ba0.285Ga0.859Al0.141O3-δ | -1.431 |  | La0.78Sr0.22Ga0.805Ti0.195O3-δ | -1.432 |
| Pr0.715Ba0.285Ga0.858Ti0.142O3-δ | -1.396 |  | La0.785Sr0.215Ga0.793Ti0.207O3-δ | -1.418 |
| Pr0.715Ba0.285Ga0.857Al0.143O3-δ | -1.433 |  | La0.784Sr0.216Ga0.808Ti0.192O3-δ | -1.434 |
| Pr0.715Ba0.285Ga0.855Ti0.145O3-δ | -1.416 |  | La0.783Sr0.217Ga0.811Al0.189O3-δ | -1.439 |
| Pr0.715Ba0.285Ga0.854Al0.146O3-δ | -1.401 |  | La0.781Sr0.219Ga0.801Al0.199O3-δ | -1.419 |
| Pr0.715Ba0.285Ga0.84Ti0.16O3-δ | -1.408 |  | La0.779Sr0.221Ga0.781Ti0.219O3-δ | -1.422 |
| Pr0.715Ba0.285Ga0.843Ti0.157O3-δ | -1.409 |  | La0.778Sr0.222Ga0.808Ti0.192O3-δ | -1.428 |
| Pr0.715Ba0.285Ga0.79Sc0.21O3-δ | -1.413 |  | La0.76Ba0.24Ga0.82Sc0.18O3-δ | -1.440 |
| Pr0.714Ba0.286Ga0.862Ti0.138O3-δ | -1.435 |  | La0.75Ba0.25Ga0.822Sc0.178O3-δ | -1.406 |
| Pr0.714Ba0.286Ga0.862Al0.138O3-δ | -1.395 |  | La0.74Ba0.26Ga0.89Ti0.11O3-δ | -1.445 |
| Pr0.714Ba0.286Ga0.821Sc0.179O3-δ | -1.436 |  | La0.74Ba0.26Ga0.88Ti0.12O3-δ | -1.388 |
| Pr0.713Ba0.287Ga0.8Sc0.2O3-δ | -1.432 |  | La0.74Ba0.26Ga0.884Ti0.116O3-δ | -1.402 |
| Pr0.713Ba0.287Ga0.858Ti0.142O3-δ | -1.407 |  | La0.74Ba0.26Ga0.873Ti0.127O3-δ | -1.372 |
| Pr0.713Ba0.287Ga0.832Ti0.168O3-δ | -1.429 |  | La0.74Ba0.26Ga0.866Ti0.134O3-δ | -1.426 |
| Pr0.713Ba0.287Ga0.82Sc0.18O3-δ | -1.421 |  | La0.74Ba0.26Ga0.865Ti0.135O3-δ | -1.414 |
| Pr0.712Ba0.288Ga0.872Al0.128O3-δ | -1.441 |  | La0.74Ba0.26Ga0.862Ti0.138O3-δ | -1.437 |
| Pr0.712Ba0.288Ga0.871Al0.129O3-δ | -1.376 |  | La0.74Ba0.26Ga0.84Sc0.16O3-δ | -1.430 |
| Pr0.712Ba0.288Ga0.853Al0.147O3-δ | -1.403 |  | La0.74Ba0.26Ga0.832Sc0.168O3-δ | -1.394 |
| Pr0.712Ba0.288Ga0.851Al0.149O3-δ | -1.394 |  | La0.74Ba0.26Ga0.831Sc0.169O3-δ | -1.395 |
| Pr0.712Ba0.288Ga0.849Al0.151O3-δ | -1.426 |  | La0.74Ba0.26Ga0.829Sc0.171O3-δ | -1.401 |
| Pr0.711Ba0.289Ga0.823Sc0.177O3-δ | -1.439 |  | La0.74Ba0.26Ga0.821Sc0.179O3-δ | -1.369 |
| Pr0.711Ba0.289Ga0.87Al0.13O3-δ | -1.362 |  | La0.745Ba0.255Ga0.86Ti0.14O3-δ | -1.433 |
| Pr0.711Ba0.289Ga0.86Al0.14O3-δ | -1.419 |  | La0.742Ba0.258Ga0.89Ti0.11O3-δ | -1.446 |
| Pr0.711Ba0.289Ga0.859Ti0.141O3-δ | -1.416 |  | La0.741Ba0.259Ga0.87Al0.13O3-δ | -1.416 |
| Pr0.711Ba0.289Ga0.856Al0.144O3-δ | -1.437 |  | La0.73Ba0.27Ga0.88Ti0.12O3-δ | -1.440 |
| Pr0.711Ba0.289Ga0.851Al0.149O3-δ | -1.434 |  | La0.73Ba0.27Ga0.875Ti0.125O3-δ | -1.424 |
| Pr0.711Ba0.289Ga0.792Sc0.208O3-δ | -1.412 |  | La0.739Ba0.261Ga0.871Al0.129O3-δ | -1.430 |
| Pr0.709Ba0.291Ga0.864Al0.136O3-δ | -1.439 |  | La0.738Ba0.262Ga0.885Ti0.115O3-δ | -1.416 |
| Pr0.705Ba0.295Ga0.859Ti0.141O3-δ | -1.432 |  | La0.737Ba0.263Ga0.863Ti0.137O3-δ | -1.445 |
| Pr0.69Ba0.31Ga0.86Ti0.14O3-δ | -1.432 |  | La0.737Ba0.263Ga0.832Sc0.168O3-δ | -1.398 |
| Pr0.69Ba0.31Ga0.862Ti0.138O3-δ | -1.435 |  | La0.737Ba0.263Ga0.831Sc0.169O3-δ | -1.398 |
| Pr0.69Ba0.31Ga0.859Ti0.141O3-δ | -1.406 |  | La0.736Ba0.264Ga0.87Al0.13O3-δ | -1.417 |
| Pr0.69Ba0.31Ga0.82Sc0.18O3-δ | -1.399 |  | La0.735Ba0.265Ga0.88Ti0.12O3-δ | -1.396 |
| Pr0.697Ba0.303Ga0.82Sc0.18O3-δ | -1.450 |  | La0.735Ba0.265Ga0.887Ti0.113O3-δ | -1.424 |
| Pr0.695Ba0.305Ga0.871Al0.129O3-δ | -1.399 |  | La0.735Ba0.265Ga0.884Ti0.116O3-δ | -1.410 |
| Pr0.685Ba0.315Ga0.864Ti0.136O3-δ | -1.412 |  | La0.735Ba0.265Ga0.87Ti0.13O3-δ | -1.434 |
| La0.8Sr0.2Ga0.818Al0.182O3-δ | -1.447 |  | La0.735Ba0.265Ga0.876Ti0.124O3-δ | -1.380 |
| La0.8Sr0.2Ga0.815Al0.185O3-δ | -1.419 |  | La0.735Ba0.265Ga0.865Ti0.135O3-δ | -1.422 |
| La0.8Sr0.2Ga0.813Al0.187O3-δ | -1.436 |  | La0.735Ba0.265Ga0.84Sc0.16O3-δ | -1.438 |
| La0.8Sr0.2Ga0.811Al0.189O3-δ | -1.353 |  | La0.735Ba0.265Ga0.82Sc0.18O3-δ | -1.425 |
| La0.8Sr0.2Ga0.809Ti0.191O3-δ | -1.442 |  | La0.735Ba0.265Ga0.823Sc0.177O3-δ | -1.372 |
| La0.8Sr0.2Ga0.808Ti0.192O3-δ | -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 |
| --- | --- | --- | --- |
| CH2-CO-NH-CS | 2.691 | NH-CO-CS-CO | 1.441 |
| CH2-CS-C6H4-O | 2.041 | CO-C6H4-C6H4-C6H4 | 2.993 |
| C6H4-C6H4-C4H2S-CS | 1.807 | CH2-CH2-C4H2S-O | 4.186 |
| CO-O-C4H2S-CS | 1.918 | NH-CS-CO-CS | 1.512 |
| C6H4-CS-C4H2S-O | 1.930 | CH2-C6H4-CS-O | 2.729 |
| CO-C6H4-O-CS | 2.772 | CH2-CO-C4H2S-CS | 1.647 |
| C6H4-O-CS-C4H2S | 2.537 | C4H2S-C4H2S-C4H2S-O | 2.267 |
| C6H4-C4H2S-C6H4-C4H2S | 2.645 | CO-C4H2S-C6H4-CS | 1.708 |
| NH-C4H2S-CO-C4H2S | 2.678 | CH2-C6H4-NH-O | 4.141 |
| CH2-NH-C4H2S-CS | 2.063 | NH-CS-NH-CS | 2.491 |
| NH-C6H4-CO-C6H4 | 3.042 | CH2-NH-CS-NH | 4.019 |
| NH-CO-CS-C4H2S | 1.701 | NH-C4H2S-C4H2S-CO | 2.521 |
| CO-C6H4-O-C4H2S | 3.410 | CH2-C4H2S-CS-O | 2.659 |
| C6H4-CS-C4H2S-CS | 1.332 | NH-CO-C4H2S-O | 3.567 |
| CH2-C4H2S-NH-C4H2S | 3.092 | CH2-C4H2S-C6H4-O | 3.375 |
| CH2-C4H2S-C6H4-C4H2S | 2.872 | C6H4-C6H4-C6H4-C4H2S | 3.046 |
| CH2-NH-C6H4-CO | 3.226 | NH-C6H4-CO-O | 3.667 |
| CO-C6H4-C4H2S-CS | 1.699 | NH-C4H2S-CO-O | 3.840 |
| C6H4-C6H4-CS-O | 2.623 | NH-CS-NH-C6H4 | 3.426 |
| CH2-NH-C4H2S-C6H4 | 2.951 | CO-CS-O-CS | 1.532 |
| NH-C4H2S-C4H2S-CH2 | 2.919 | CH2-NH-CH2-CS | 2.141 |
| CH2-C4H2S-C6H4-CS | 1.841 | CH2-CH2-NH-C6H4 | 4.005 |
| CH2-NH-CS-C6H4 | 2.737 | C4H2S-C4H2S-C4H2S-CS | 1.686 |
| CH2-C6H4-C4H2S-C6H4 | 2.960 | CH2-C6H4-C6H4-O | 3.823 |
| NH-CO-C4H2S-C6H4 | 3.244 | CH2-CO-C6H4-CS | 1.741 |
| NH-C4H2S-NH-CS | 3.123 | CO-C6H4-C6H4-CS | 1.800 |
| CO-C6H4-C4H2S-O | 2.590 | CH2-CH2-CH2-CS | 2.315 |
| NH-C4H2S-O-C4H2S | 3.878 | CH2-C6H4-CH2-O | 4.867 |
| CH2-NH-CH2-CO | 3.842 | CH2-O-CO-O | 6.933 |
| NH-CO-NH-C6H4 | 4.455 | NH-C6H4-CS-C6H4 | 1.924 |
| CH2-C6H4-NH-CS | 2.960 | CH2-CO-C6H4-O | 3.499 |
| CH2-CH2-CH2-O | 6.863 | CH2-NH-C4H2S-NH | 3.701 |
| CH2-CS-CH2-O | 2.411 | CH2-C6H4-CO-O | 4.293 |
| NH-C6H4-C6H4-O | 3.619 | CH2-C6H4-CH2-CS | 2.354 |
| CH2-C4H2S-NH-CS | 3.025 | CH2-C6H4-NH-C6H4 | 3.570 |
| CH2-C6H4-O-C4H2S | 4.281 | C6H4-C4H2S-C6H4-O | 2.904 |
| CH2-CH2-CO-C6H4 | 3.407 | C6H4-C4H2S-O-CS | 2.824 |
| CO-C4H2S-C4H2S-CS | 1.599 | CH2-C4H2S-C4H2S-CS | 1.762 |
| CH2-C6H4-O-C6H4 | 4.132 | CH2-CO-CH2-O | 4.348 |
| CO-C4H2S-C6H4-O | 2.740 | C6H4-C4H2S-C4H2S-C4H2S | 2.321 |
| CO-C4H2S-CO-O | 2.930 | CH2-C4H2S-NH-O | 3.964 |
| CH2-CS-C4H2S-O | 2.028 | CH2-CO-C6H4-C4H2S | 3.001 |
| CH2-O-C4H2S-C6H4 | 3.240 | NH-CO-O-C4H2S | 4.288 |
| CH2-C4H2S-CO-C4H2S | 3.095 | CH2-C4H2S-CO-O | 3.772 |
| CO-C6H4-CO-O | 2.979 | CH2-CS-C6H4-NH | 2.063 |
| CH2-CH2-CO-C4H2S | 3.376 | CO-O-C6H4-CS | 1.932 |
| CH2-CO-CS-C6H4 | 1.754 | NH-CO-C4H2S-CS | 1.773 |
| CH2-CS-CO-O | 1.599 | NH-CO-O-CS | 2.917 |
| NH-C4H2S-NH-C4H2S | 3.515 | CH2-NH-CS-CO | 2.093 |
| C6H4-CS-C6H4-CS | 1.511 | CH2-CO-C4H2S-O | 3.320 |
| CH2-C6H4-CH2-C6H4 | 4.691 | CH2-CH2-C6H4-O | 4.351 |
| CH2-C4H2S-O-CS | 3.061 | CH2-C6H4-CS-C6H4 | 1.889 |
| CO-C6H4-C6H4-C4H2S | 2.705 | CO-C6H4-CO-C6H4 | 2.826 |
| CH2-CH2-NH-C4H2S | 3.931 | CH2-C4H2S-CH2-O | 4.313 |
| CH2-CH2-CO-O | 5.794 | CH2-NH-C4H2S-CO | 2.987 |
| CH2-CO-CS-C4H2S | 1.651 | CH2-NH-C6H4-NH | 3.392 |
| CH2-NH-CH2-NH | 5.942 | NH-CS-O-CS | 2.557 |
| C6H4-CS-C4H2S-C4H2S | 1.728 | CH2-C6H4-O-CS | 3.054 |
| NH-CO-C6H4-CS | 1.836 | NH-CS-C4H2S-O | 2.562 |
| NH-CO-NH-CO | 4.829 | CO-C6H4-C6H4-O | 2.965 |
| C4H2S-C4H2S-O-CS | 2.588 | CH2-NH-CH2-C4H2S | 4.226 |
| NH-CS-NH-O | 3.988 | C4H2S-CS-O-CS | 1.912 |
| CO-O-C4H2S-O | 4.016 | CO-C4H2S-C6H4-C4H2S | 2.505 |
| CH2-O-C4H2S-O | 4.150 | CO-C4H2S-C4H2S-C4H2S | 2.080 |
| NH-O-CO-O | 6.731 | CH2-NH-CS-C4H2S | 2.571 |
| CH2-CO-O-CS | 2.705 | NH-O-CS-O | 4.333 |
| CH2-O-C6H4-O | 3.859 | CH2-NH-CH2-C6H4 | 4.318 |
| NH-C6H4-NH-O | 3.571 | CH2-C6H4-CO-C4H2S | 3.144 |
| CH2-CH2-C6H4-C4H2S | 3.526 | CH2-O-CH2-O | 6.436 |
| NH-C4H2S-CS-O | 2.612 | CO-C6H4-C4H2S-C4H2S | 2.361 |
| C6H4-C6H4-C4H2S-C4H2S | 2.615 | CH2-CO-CS-O | 2.161 |
| NH-C4H2S-C6H4-C4H2S | 2.584 | NH-CO-CS-O | 2.557 |
| CO-C4H2S-C4H2S-O | 2.360 | CH2-CO-CS-CO | 1.278 |
| NH-C4H2S-CO-CS | 1.633 | CH2-NH-C6H4-C4H2S | 3.176 |
| NH-C4H2S-C4H2S-C4H2S | 2.344 | NH-CS-C6H4-CS | 1.639 |
| CH2-CH2-CH2-C6H4 | 5.108 | NH-C6H4-C6H4-CH2 | 3.569 |
| NH-C4H2S-O-CS | 2.550 | NH-CO-NH-CS | 2.941 |
| CH2-NH-CS-O | 4.240 | NH-C4H2S-C4H2S-CS | 1.764 |
| CH2-CO-O-C4H2S | 4.022 | NH-C6H4-NH-C6H4 | 3.313 |
| CO-C6H4-CS-C6H4 | 1.753 | NH-C6H4-NH-C4H2S | 3.149 |
| NH-CS-C4H2S-CS | 1.614 | CH2-C6H4-C6H4-C4H2S | 3.190 |
| NH-CO-C6H4-C4H2S | 3.238 | CH2-C4H2S-CS-C4H2S | 1.802 |
| NH-C4H2S-CS-C4H2S | 1.882 | CO-NH-CO-C6H4 | 3.710 |
| C6H4-C4H2S-O-C4H2S | 3.310 | CH2-CS-CO-CS | 1.492 |
| C6H4-C6H4-C6H4-CS | 1.879 | CH2-CH2-NH-CS | 3.375 |
| CH2-C4H2S-CH2-C4H2S | 4.109 | CH2-C4H2S-C4H2S-O | 2.817 |
| CO-CS-CO-O | 1.477 | CH2-CO-NH-C4H2S | 4.130 |
| CO-C6H4-C4H2S-C6H4 | 2.546 | CH2-CH2-CO-CS | 1.425 |
| CH2-CH2-CH2-CH2 | 8.828 | NH-C6H4-C6H4-C4H2S | 2.930 |
| NH-CO-C6H4-C6H4 | 3.656 | CH2-C6H4-C4H2S-CS | 1.834 |
| NH-CO-CS-C6H4 | 1.721 | C6H4-O-CS-O | 3.903 |
| CO-C6H4-CS-C4H2S | 1.787 | CH2-O-NH-CO | 5.357 |
| CH2-CO-CH2-CO | 3.761 | NH-C6H4-C4H2S-C6H4 | 2.753 |
| CO-O-C6H4-O | 4.193 | C6H4-O-C4H2S-O | 4.061 |
| NH-CO-C4H2S-CO | 3.029 | NH-C6H4-O-C4H2S | 3.606 |
| CH2-C6H4-C4H2S-C4H2S | 2.737 | CH2-NH-CO-CS | 1.827 |
| CO-C6H4-CO-C4H2S | 2.867 | CH2-NH-C6H4-O | 3.538 |
| CH2-C6H4-CO-CS | 1.735 | C6H4-C6H4-C6H4-C6H4 | 3.307 |
| CH2-CH2-C6H4-CS | 1.965 | CH2-CO-NH-C6H4 | 4.296 |
| NH-C4H2S-C6H4-CS | 1.850 | CH2-CH2-C4H2S-C4H2S | 3.124 |
| CH2-NH-O-C6H4 | 4.520 | CH2-NH-CH2-O | 5.758 |
| CH2-C6H4-C6H4-C6H4 | 3.533 | NH-C6H4-C6H4-C6H4 | 3.145 |
| CH2-O-NH-O | 6.258 | C6H4-CS-O-CS | 1.914 |
| CH2-CH2-C4H2S-CS | 1.939 | CO-C4H2S-CS-O | 2.246 |
| NH-CO-NH-C4H2S | 4.069 | NH-C6H4-C4H2S-C4H2S | 2.587 |
| CH2-C4H2S-CH2-CS | 2.322 | CH2-CH2-CH2-NH | 6.207 |
| NH-CO-NH-O | 5.284 | CH2-CO-NH-CO | 4.232 |
| CO-C6H4-CS-O | 2.340 | NH-CS-C6H4-O | 2.700 |
| CH2-CH2-O-NH | 6.746 | CO-C4H2S-CO-C4H2S | 2.765 |
| CH2-CO-CH2-C4H2S | 3.997 | NH-C6H4-O-CS | 2.945 |
| C6H4-O-C6H4-O | 4.085 | CH2-C4H2S-CO-CS | 1.532 |
| CH2-O-CS-O | 3.958 | CH2-CO-O-C6H4 | 4.756 |
| NH-CO-C6H4-O | 4.072 | C4H2S-C4H2S-C4H2S-C4H2S | 2.019 |
| C4H2S-O-C4H2S-O | 4.103 | CO-C6H4-O-C6H4 | 3.441 |
| CH2-NH-CO-C6H4 | 3.951 | CH2-CH2-CH2-C4H2S | 4.506 |
| CH2-C4H2S-O-C4H2S | 3.773 | NH-CO-O-C6H4 | 4.926 |
| CH2-CO-O-CO | 4.582 | CO-C4H2S-O-CS | 2.823 |
| CH2-CO-C4H2S-C6H4 | 3.020 | C6H4-C4H2S-C4H2S-O | 2.605 |
| CH2-CO-C6H4-CO | 2.795 | CH2-CO-C4H2S-C4H2S | 2.596 |
| NH-C4H2S-C4H2S-O | 2.834 | CH2-CO-CH2-CS | 2.174 |
| C6H4-C4H2S-C6H4-CS | 1.806 | NH-C6H4-C4H2S-CS | 1.856 |
| CH2-C6H4-CS-C4H2S | 1.845 | CH2-C4H2S-C4H2S-C4H2S | 2.328 |
| C6H4-C4H2S-CS-C4H2S | 1.740 | NH-C6H4-CS-O | 2.830 |
| C4H2S-O-CS-O | 3.820 | NH-C6H4-CO-C4H2S | 2.887 |
| CH2-CS-NH-O | 3.256 | CO-C4H2S-CO-CS | 1.447 |
| CH2-C6H4-CH2-C4H2S | 4.409 | NH-CS-CO-O | 2.267 |
| CO-O-CS-O | 3.374 | CH2-CS-NH-CS | 2.051 |
| NH-C6H4-O-C6H4 | 3.875 | C6H4-C6H4-C4H2S-O | 2.951 |
| CH2-C6H4-CO-C6H4 | 3.186 | CH2-CO-C4H2S-CO | 2.750 |
| NH-CO-O-CO | 5.163 | CH2-NH-CO-C4H2S | 3.946 |
| CO-C4H2S-CS-C4H2S | 1.633 | CH2-C6H4-C6H4-CS | 1.898 |
| CH2-CS-O-CS | 2.214 | CH2-C6H4-NH-C4H2S | 3.464 |
| C4H2S-CS-C4H2S-O | 1.860 | CH2-CO-C6H4-C6H4 | 3.215 |
| CO-C4H2S-O-C4H2S | 3.325 | CH2-CH2-CS-O | 3.309 |
| C6H4-CS-C6H4-O | 1.915 | NH-C4H2S-CS-C6H4 | 1.964 |
| NH-O-C6H4-O | 3.916 | CH2-NH-O-C4H2S | 4.294 |
| CH2-CO-CH2-C6H4 | 4.257 | C6H4-C6H4-C6H4-O | 3.396 |
| CH2-NH-O-CS | 3.231 | NH-C6H4-CO-CS | 1.760 |
| CH2-NH-C4H2S-O | 3.881 | CH2-CH2-C6H4-C6H4 | 4.020 |
| CH2-CS-C4H2S-CS | 1.319 | CH2-CS-CH2-CS | 1.890 |
| CO-C6H4-CO-CS | 1.648 | NH-C6H4-C6H4-CS | 1.917 |
| CH2-CH2-CH2-CO | 4.112 | CH2-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 | H2流量/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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |