

# 物理学报

第 73 卷 第 6 期 2024 年 3 月 20 日

## 目 次

### 特邀综述

- 064201 非互易拓扑光子学 ..... 王子尧 陈福家 郁翔 高振 杨怡豪

### 专题: 缺陷与掺杂对物性的调控

#### 综述

- 063101 钙钛矿太阳能电池材料缺陷对器件性能与稳定性的影响 ..... 王静 高姗 段香梅 尹万健

- 066105 半导体缺陷的电子结构计算方法研究进展 ..... 李晨慧 张陈 蔡雪芬 张才鑫 袁嘉怡 邓惠雄

- 067401 Kagome 超导体  $AV_3Sb_5$  ( $A = K, Rb, Cs$ ) 的掺杂效应 ..... 李永恺 刘锦锦 张鑫 朱鹏 杨柳 张钰琪 吴黄宇 王秩伟

#### 研究论文

- 066104 过渡金属元素掺杂对磁铁矿磁矩及磁各向异性的调控 ..... 任延英 李雅宁 柳洪盛 徐楠 郭坤 徐朝辉 陈鑫 高峻峰

- 067101 元素掺杂对储氢容器用高强钢性能影响的第一性原理和分子动力学模拟 ..... 胡庭赫 李直昊 张千帆

### 专题: 生物分子模拟中的机器学习

#### 综述

- 068702 分子体系自由能地貌图的变分分析及 AI 算法实现 ..... 杜泊船 田圆

- 069301 蛋白质计算中的机器学习 ..... 张嘉晖

### 总论

- 060201 基于最优控制理论的国产光抽运小铯钟频率控制算法 ..... 宋会杰 董绍武 王翔 姜萌 章宇 郭栋 张继海

- 060301 连续变量量子密钥分发系统中动态偏振控制研究 ..... 张光伟 白建东 颜琦 靳晶晶 张永梅 刘文元

- 060302 基于硬件同步的四态离散调制连续变量量子密钥分发 ..... 张云杰 王旭阳 张瑜 王宁 贾雁翔 史玉琪 卢振国 邹俊 李永民

- 060701 激光脉冲啁啾影响双色激光场诱导气体产生太赫兹辐射特性的理论研究 ..... 李翰楠 彭滟

- 060702 数字型太赫兹带通滤波器的逆向设计及优化 ..... 居学尉 张林烽 黄峰 朱国锋 李淑锦 陈燕青 王嘉勋 钟舜聪 陈盈 王向峰

### 核物理学

- 062101 强激光场对原子核  $\alpha$  衰变的影响 ..... 张凯林 韩胜贤 岳生俊 刘作业 胡碧涛

- 062102 基于实稳定方法的原子核单粒子共振相对论 Hartree-Fock 模型 ..... 杨威 丁士缘 孙保元

- 062301 原子核  $\beta$  衰变寿命经验公式 ..... 夏金戈 李伟峰 方基宇 牛中明

### 原子和分子物理学

- 063201 溶液法原位大面积制备钙钛矿光电薄膜成膜的同步辐射可视化结晶过程研究 ..... 杨迎国 冯尚蕾 李丽娜

- 063401 氧化钪 ( $Sc_2O_3$ ) 的热漫散射强度解析 ..... 王瑞刚 刘泽朋 香莲 孙勇

### 电磁学、光学、声学、传热学、经典力学和流体动力学

- 064202 基于纳米金属阵列天线的石墨烯/硅近红外探测器 ..... 张逸飞 刘媛 梅家栋 王军转 王肖沫 施毅

- 064203** 基于多尺度特征增强的合成孔径光学图像复原 … 张银胜 童俊毅 陈戈 单梦姣 王硕洋 单慧琳  
**064301** 基于亥姆霍兹共振的超薄弧形声学超表面地毯斗篷 ..... 隋玉梅 何兆剑 毕仁贵 孔鹏 吴吉恩 赵鹤平 邓科  
**064701** 微通道中一类生物流体在高 Zeta 势下的电渗流及传热特性 ..... 慕江勇 崔继峰 陈小刚 赵毅康 田袆琳 于欣如 袁满玉

### 气体、等离子体和放电物理

- 065201** 基于极限梯度提升的完美匹配单层智能算法实现航空瞬变电磁问题高效吸收 ..... 冯乃星 王欢 朱子贤 董纯志 李宏杨 张玉贤 杨利霞 黄志祥  
**065202** HL-2A 装置高  $\beta_N$  双输运垒实验的集成分析 ..... 李正吉 陈伟 孙爱萍 于利明 王卓 陈佳乐 许健强 李继全 石中兵 蒋敏 李永高 何小雪 杨曾辰 李鉴  
**065203** 基于超级电容器的充放电电路系统研制及其在 EAST 限制器探针测量中的应用 ..... 张问博 刘少承 廖亮 魏文峯 李乐天 王亮 颜宁 钱金平 臧庆

### 凝聚物质: 结构、力学和热学性质

- 066101** 向列相液晶分子结构与黏度关系研究及 BPNN-QSAR 模型建立 ..... 陈红梅 李世伟 李凯靖 张智勇 陈浩 王婷婷  
**066102** 大晶粒  $UO_2$  燃料裂变气体释放行为相场模拟研究 ..... 刘东昆 王庆宇 张田 周羽 王翔  
**066103** 基于 55 nm DICE 结构的单粒子翻转效应模拟研究 ..... 张幸 刘玉林 李刚 燕少安 肖永光 唐明华  
**066601** 非均匀流体的体积黏度: Maxwell 弛豫模型 ..... 孙宗利 康艳霜 张君霞  
**066701** 紧凑型冷原子高分辨成像系统光学设计 ..... 沈晓阳 成一灏 夏林

### 凝聚物质: 电子结构、电学、磁学和光学性质

- 067301** 基于  $GaN/(BA)_2PbI_4$  异质结的自供电双模式紫外探测器 ..... 张盛源 夏康龙 张茂林 边昂 刘增 郭宇锋 唐为华  
**067501**  $Mn_3Sn$  薄膜磁相变的输运表征 ..... 谭碧 高栋 邓登福 陈姝瑶 毕磊 刘冬华 刘涛  
**067601** 高频率分辨的金刚石氮-空位色心宽频谱成像技术 ..... 中圆圆 王博 柯冬倩 郑斗斗 李中豪 温焕飞 郭浩 李鑫 唐军 马宗敏 李艳君 伊戈尔·费拉基米罗维奇·雅明斯基 刘俊

### 物理学交叉学科及有关科学技术领域

- 068401** 双级 PIN 限幅器的微波脉冲响应机理及规律 ..... 高铭萱 张洋 张军  
**068501** 基于超导单光子探测器的红外光学系统噪声分析和优化 ..... 周飞 陈奇 刘浩 戴越 魏晨 袁杭 王昊 涂学凑 康琳 贾小氢 赵清源 陈健 张蜡宝 吴培亨  
**068502** 3D NAND 闪存中氟攻击问题引起的字线漏电的改进 ..... 方语萱 夏志良 杨涛 周文犀 霍宗亮  
**068701** 用于多通道单分子定位的高精度图像配准方法 **封面文章** ..... 林丹樱 龚振权 黄黎琳 聂梦娇 于斌 屈军乐  
**068801** 溶液法制备二维钙钛矿层提高甲脒碘化铅钙钛矿太阳能电池稳定性 ..... 刘思雯 任立志 金博文 宋欣 吴聪聪

文章图片的彩色效果详见网刊



扫码阅读  
电子版

# ACTA PHYSICA SINICA

Vol. 73, No. 6, March 20, 2024

## CONTENTS

### INVITED REVIEW

- 064201 Non-reciprocal topological photonics

*Wang Zi-Yao Chen Fu-Jia Xi Xiang Gao Zhen Yang Yi-Hao*

### SPECIAL TOPIC—Modification of material properties by defects and dopants REVIEW

- 063101 Influence of defect in perovskite solar cell materials on device performance and stability

*Wang Jing Gao Shan Duan Xiang-Mei Yin Wan-Jian*

- 066105 A review of first-principles calculation methods for defects in semiconductors

*Li Chen-Hui Zhang Chen Cai Xue-Fen Zhang Cai-Xin Yuan Jia-Yi Deng Hui-Xiong*

- 067401 Doping effects of Kagome superconductor  $AV_3Sb_5$  ( $A = K, Rb, Cs$ )

*Li Yong-Kai Liu Jin-Jin Zhang Xin Zhu Peng Yang Liu Zhang Yu-Qi Wu Huang-Yu Wang Zhi-Wei*

### ARTICLE

- 066104 Regulation of magnetic moment and magnetic anisotropy of magnetite by doping transition metal elements

*Ren Yan-Ying Li Ya-Ning Liu Hong-Sheng Xu Nan Guo Kun Xu Zhao-Hui Chen Xin Gao Jun-Feng*

- 067101 First principles and molecular dynamics simulations of effect of dopants on properties of high strength steel for hydrogen storage vessels

*Hu Ting-He Li Zhi-Hao Zhang Qian-Fan*

### SPECIAL TOPIC—Machine learning in biomolecular simulations

#### REVIEW

- 068702 Variational analysis and AI algorithm implementation of free energy landscapes of molecular system

*Du Bo-Chuan Tian Pu*

- 069301 Machine learning for *in silico* protein research

*Zhang Jia-Hui*

### GENERAL

- 060201 Frequency control algorithm of domestic optically pumped small cesium clock based on optimal control theory

*Song Hui-Jie Dong Shao-Wu Wang Xiang Jiang Meng Zhang Yu Guo Dong Zhang Ji-Hai*

- 060301 Research on dynamic polarization control in continuous variable quantum key distribution systems

*Zhang Guang-Wei Bai Jian-Dong Jie Qi Jin Jing-Jing Zhang Yong-Mei Liu Wen-Yuan*

- 060302 Four-state discrete modulation continuous variable quantum key distribution based on hardware synchronization

*Zhang Yun-Jie Wang Xu-Yang Zhang Yu Wang Ning Jia Yan-Xiang Shi Yu-Qi Lu Zhen-Guo Zou Jun Li Yong-Min*

- 060701 Theoretical study of influence of laser pulse chirp on terahertz emission characteristics of gas induced by two-color laser field

*Li Han-Nan Peng Yan*

(Continued)

- 060702 Reverse design and optimization of digital terahertz bandpass filters  
*Ju Xue-Wei Zhang Lin-Feng Huang Feng Zhu Guo-Feng Li Shu-Jin Chen Yan-Qing Wang Jia-Xun Zhong Shun-Cong Chen Ying Wang Xiang-Feng*

## NUCLEAR PHYSICS

- 062101 Influence of strong laser field on nuclear  $\alpha$  decay  
*Zhang Kai-Lin Han Sheng-Xian Yue Sheng-Jun Liu Zuo-Ye Hu Bi-Tao*
- 062102 Relativistic Hartree-Fock model of nuclear single-particle resonances based on real stabilization method  
*Yang Wei Ding Shi-Yuan Sun Bao-Yuan*
- 062301 An empirical formula of nuclear  $\beta$ -decay half-lives  
*Xia Jin-Ge Li Wei-Feng Fang Ji-Yu Niu Zhong-Ming*

## ATOMIC AND MOLECULAR PHYSICS

- 063201 Solution slot-die coating perovskite film crystalline growth observed by *in situ* GIWAXS/GISAXS  
*Yang Ying-Guo Feng Shang-Lei Li Li-Na*
- 063401 Analysis of thermal diffuse scattering intensity of scandium oxide ( $\text{Sc}_2\text{O}_3$ )  
*Wang Rui-Gang Liu Ze-Peng Xiang-Lian Sun Yong*

## ELECTROMAGNETISM, OPTICS, ACOUSTICS, HEAT TRANSFER, CLASSICAL MECHANICS, AND FLUID DYNAMICS

- 064202 Quaternary nanoparticle array antenna for graphene/silicon near-infrared detector  
*Zhang Yi-Fei Liu Yuan Mei Jia-Dong Wang Jun-Zhuan Wang Xiao-Mu Shi Yi*
- 064203 Synthetic aperture optical image restoration based on multi-scale feature enhancement  
*Zhang Yin-Sheng Tong Jun-Yi Chen Ge Shan Meng-Jiao Wang Shuo-Yang Shan Hui-Lin*
- 064301 Ultrathin acoustic metasurface carpet cloaking based on Helmholtz resonances  
*Sui Yu-Mei He Zhao-Jian Bi Ren-Gui Kong Peng Wu Ji-En Zhao He-Ping Deng Ke*
- 064701 Electroosmotic flow and heat transfer characteristics of a class of biofluids in microchannels at high Zeta potential  
*Mu Jiang-Yong Cui Ji-Feng Chen Xiao-Gang Zhao Yi-Kang Tian Yi-Lin Yu Xin-Ru Yuan Man-Yu*

## PHYSICS OF GASES, PLASMAS, AND ELECTRIC DISCHARGES

- 065201 Intelligent algorithm of extreme gradient boosting based perfectly matched monolayer and its efficient absorption on airborne transient electromagnetics problems  
*Feng Nai-Xing Wang Huan Zhu Zi-Xian Dong Chun-Zhi Li Hong-Yang Zhang Yu-Xian Yang Li-Xia Huang Zhi-Xiang*
- 065202 Integrated analysis of high- $\beta_N$  double transport barriers scenario on HL-2A  
*Li Zheng-Ji Chen Wei Sun Ai-Ping Yu Li-Ming Wang Zhuo Chen Jia-Le Xu Jian-Qiang Li Ji-Quan Shi Zhong-Bing Jiang Min Li Yong-Gao He Xiao-Xue Yang Zeng-Chen Li Jian*
- 065203 Development of charge-discharge circuitry based on supercapacitor and its application to limiter probe diagnostics in EAST  
*Zhang Wen-Bo Liu Shao-Cheng Liao Liang Wei Wen-Yin Li Le-Tian Wang Liang Yan Ning Qian Jin-Ping Zang Qing*

## CONDENSED MATTER: STRUCTURAL, MECHANICAL, AND THERMAL PROPERTIES

- 066101 Molecules structure and viscosity relationship of nematic liquid crystal and BPNN-QSAR model  
*Chen Hong-Mei Li Shi-Wei Li Kai-Jing Zhang Zhi-Yong Chen Hao Wang Ting-Ting*
- 066102 Phase-field simulation on fission gas release behavior of large grain  $\text{UO}_2$  fuel  
*Liu Dong-Kun Wang Qing-Yu Zhang Tian Zhou Yu Wang Xiang*

(Continued)

- 066103 Three-dimensional numerical simulation of single event upset effect based on 55 nm DICE latch unit  
*Zhang Xing Liu Yu-Lin Li Gang Yan Shao-An Xiao Yong-Guang Tang Ming-Hua*
- 066601 Volume viscosity of inhomogeneous fluids: a Maxwell relaxation model  
*Sun Zong-Li Kang Yan-Shuang Zhang Jun-Xia*
- 066701 Design of compact high resolution imaging system for cold atom experiments  
*Shen Xiao-Yang Cheng Yi-Hao Xia Lin*

## CONDENSED MATTER: ELECTRONIC STRUCTURE, ELECTRICAL, MAGNETIC, AND OPTICAL PROPERTIES

- 067301 Self-powered dual-mode UV detector based on GaN/(BA)<sub>2</sub>PbI<sub>4</sub> heterojunction  
*Zhang Sheng-Yuan Xia Kang-Long Zhang Mao-Lin Bian Ang Liu Zeng Guo Yu-Feng Tang Wei-Hua*
- 067501 Transport characterization of magnetic phase transition in Mn<sub>3</sub>Sn thin films  
*Tan Bi Gao Dong Deng Deng-Fu Chen Shu-Yao Bi Lei Liu Dong-Hua Liu Tao*
- 067601 High-frequency resolution diamond nitrogen-vacancy center wide-spectrum imaging technology  
*Shen Yuan-Yuan Wang Bo Ke Dong-Qian Zheng Dou-Dou Li Zhong-Hao Wen Huan-Fei Guo Hao Li Xin Tang Jun Ma Zong-Min Li Yan-Jun Igor Vladimirovich Yaminsky Liu Jun*

## INTERDISCIPLINARY PHYSICS AND RELATED AREAS OF SCIENCE AND TECHNOLOGY

- 068401 Mechanism and rule of microwave pulse response of two-stage PIN limiter  
*Gao Ming-Xuan Zhang Yang Zhang Jun*
- 068501 Noise characteristics analysis and suppression of optical system based on infrared superconducting single-photon detector  
*Zhou Fei Chen Qi Liu Hao Dai Yue Wei Chen Yuan Hang Wang Hao Tu Xue-Cou Kang Lin Jia Xiao-Qing Zhao Qing-Yuan Chen Jian Zhang La-Bao Wu Pei-Heng*
- 068502 Improvement of fluorine attack induced word-line leakage in 3D NAND flash memory  
*Fang Yu-Xuan Xia Zhi-Liang Yang Tao Zhou Wen-Xi Huo Zong-Liang*
- 068701 A high-precision image registration method for multi-channel single molecule localization  
**COVER ARTICLE**  
*Lin Dan-Ying Gong Zhen-Quan Huang Li-Lin Nie Meng-Jiao Yu Bin Qu Jun-Le*
- 068801 Preparation of two-dimensional perovskite layer by solution method for improving stability of FAPbI<sub>3</sub> perovskite solar cells  
*Liu Si-Wen Ren Li-Zhi Jin Bo-Wen Song Xin Wu Cong-Cong*

Color figures can be viewed in the online issue.



Online issue