

Artificial Intelligence Driven Optoelectronic Data Mining for Advanced High-Integration Spectral Sensing

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2024 Peking University "Boya M-Talents" International Doctoral Students Academic Forum 2024

Sub forum 2 Latest Research Report on Optoelectronic Materials



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- 1 Miniaturized Spectral Detection Background
- 2 Device Design And Implementation
- 3 Automated High-throughput Testing
- 4 AI Assisted Spectral Reconstruction
- 5 Summary and acknowledgment

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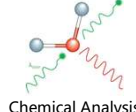
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1 Miniaturized Spectrometer Background





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◆ Applications Development




Chemical Analysis

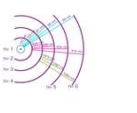


biomedicine


Traditional Application




astro observation




material science



Doran
Precision Agriculture



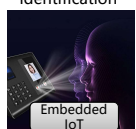
Satellite
Deep Space Exploration




Aeroplane
Geological Exploration

Cutting-edge Requirements

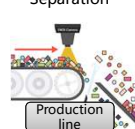
Miniaturization, Portable, Integration



Biometric Identification
Embedded IoT



Precision Medicine
Portable device



Plastics Separation
Production line


ICSE

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1 Miniaturized Spectrometer Background

◆Miniaturization Development

Traditional **Benchtop Spectral Detector**



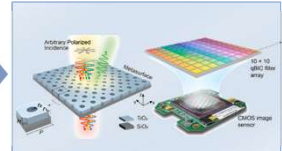
➤**Tech. Adv.:**

- High spectral resolution
- Mature optical spectroscopy techniques

➤**Perennial Problem:**

- Large and heavy optical components
- Supports only push-broom imaging

Miniaturized **Integrated Optical Structure Spectrometer**



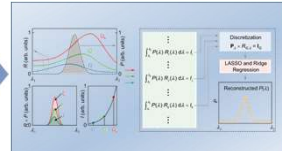
➤**Tech. Adv.:**

- Enables **snapshot imaging**
- Optical components miniaturized

➤**Perennial Problem:**

- Micro-nano optics **add cost**
- Integration challenges** in mass production.

Optical Structure Free **Micro-spectrometer**



➤**Tech. Adv.:**

- No extra micro-nano steps
- Scalable to large 2D arrays

➤**Perennial Problem:**

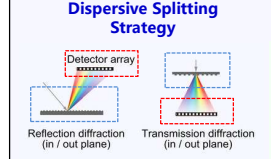
- Limited modulation, singular spectral response. Error-prone reconstruction, low accuracy.

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1 Miniaturized Spectrometer Background

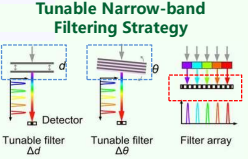
◆Technical strategy of spectrometer miniaturization

Dispersive Splitting Strategy



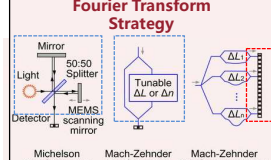
Reflection diffraction (in / out plane) / Transmission diffraction (in / out plane)

Tunable Narrow-band Filtering Strategy



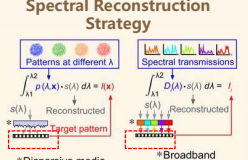
Tunable filter d / Tunable filter $\Delta\theta$ / Filter array

Fourier Transform Strategy



Mirror / 50:50 Splitter / MEMS scanning mirror / Michelson interferometer / Mach-Zehnder interferometer / Mach-Zehnder interferometer array

Spectral Reconstruction Strategy



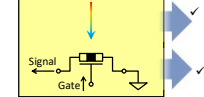
Patterns at different λ / Spectral transmissions / Reconstructed $s(\lambda)$ / Target pattern / Broadband filter array

Array detector Dependence

Micro-nano optical Dependence

Integration Limited Complicated Process

Single Point Reconstruction Spectrometer



- ✓ Optical Module Free
- ✓ Single Detector

✱ Xia FN. *Nat. Photon.* 15, 601-607 (2021)
 ✱ Sun ZP. *Science.* 378,296-299 (2022)

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1 Miniaturized Spectrometer Background

◆Basic principle of single-point reconstructed spectrometer

Math.

$$\begin{bmatrix} R_{1,1} & \dots & R_{1,n} \\ \vdots & \ddots & \vdots \\ R_{m,1} & \dots & R_{m,n} \end{bmatrix} \begin{bmatrix} S_1 \\ \vdots \\ S_n \end{bmatrix} = \begin{bmatrix} I_1 \\ \vdots \\ I_m \end{bmatrix}$$

Reconstruction

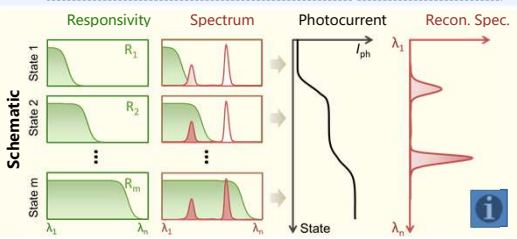
$$\begin{bmatrix} I_1 \\ \vdots \\ I_m \end{bmatrix} R^{-1} = \begin{bmatrix} S_1 \\ \vdots \\ S_n \end{bmatrix}$$

Singular Matrix -> Ill-posed Problem

Method	Pro.	Con.
Tikhonov Reg.	Suppress noise and reduce errors	Need right parameters
SVD	Stable for ill-conditioned	High computational complexity
M-P pseudo inverse	Stable for non-full rank matrices	Complexity for dense matrices
QR decomposition	Numerical stability is good	Not suitable for direct inversion
iterative	Suitable for large-scale problems	Dependent on initial values, converge slowly.

Core How to improve precision in S.P. detection?

Schematic



Responsivity R_i / Spectrum S_i / Photocurrent I_{ph} / Recon. Spec. λ_n

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1 Miniaturized Spectrometer Background

科学问题：如何实现高精度的单点探测器光谱探测？

实现内化且原位可控的光谱感知能力

二维材料带隙原位调控

化学气相沉积 / 高分辨透射电镜 / 高压液相合成

器件制备

需要丰富完整且系统的光电特征表征

高通量自动化光电测试与分析

核电极调控 / 面内应力极化调控

制备面内核电极调控光电探测原型器件

光电子发射型表征 / 光光谱响应测试

构建器件红外光电瞬态响应的物理模型

厘清电学模态调控红外光谱探测器设计理论

针对性设计的信号采集与重构算法

复合信号读出与神经网络重构

光电瞬态响应参量同步读出电路设计

复合信号高精度光谱重构算法研究

高精度近红外-短波红外光谱探测像元原型评估

基于二维材料的微型复合信号重构光谱仪研究

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2 **S.P. Spectrometer Device**

3 Automated High-throughput Testing

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5 Summary and acknowledgment

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2 S.P. Spectrometer Device

◆ Design of semi-suspended 2D MoS₂ devices.

Normalized Intensity (a.u.) vs Energy (eV) plot showing band structure evolution with strain.

◆ Wang ZL. *Nature* **514**, 470-474 (2014).
◆ Zhang X. *Nature Nanotech* **10**, 151-155 (2015).

In-plane piezoelectric control technology, based on the symmetry breaking of single-layer structures. → Strain -> band structure: **bandgap compression** and evolution towards **indirect bandgap**.

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2 S.P. Spectrometer Device

◆ Control the response cutoff wavelength

● Raman E_{2g} Mapping

● Photoelectric transport curve

◆ Liu Y. *Nat Commun.* **11**, 1151 (2020)

In-plane gate-induced lattice distortion (Raman characteristic peak shift) → Bandgap Compression → Extended Response Cutoff Wavelength

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2 S.P. Spectrometer Device

◆ Realization of WDM detection

● WDM Scheme

● Wave decomposition multiplexing detection diagram

● Mathematical procedure

V_G gradual increase → Series of photocurrents I(V_G)
Differential I(V_G) → Spectrum curve

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2 S.P. Spectrometer Device

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Experimental Results

- Photocurrent Signal
- Reconstructed Transient Spectrum

The demultiplexing of optical signals in five bands is realized in the wavelength range of 600-800 nm → **Lack of Precision**

The spectrum is encoded in the photoelectric response

Jointly influenced by sampling accuracy and algorithm accuracy

Q1 Characteristic information of photoelectric response has not been fully mined

Q2 Optimize signal sampling and design reconstruction algorithm is important

Core How to improve precision in S.P. detection?

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3 Automated High-throughput Testing

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High throughput AI experiment platform

AI design algorithm | HTP photoelectric test | ML feedback

para input

Experimental scheme

HTP preparation

- 1 八孔载架
- 2 照相系统
- 3 八通道移液器
- 4 定角旋涂仪
- 5 硅片式热台
- 6 多功能抓手

HTP characterization

- 7 机械臂
- 8 显微镜
- 9 多孔载架

HTP test

- 10 光学表征
- 11 机械臂
- 12 光电子表征

Machine learning

Material gene bank

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3 Automated High-throughput Testing



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#3 高通量表征

High-throughput charac

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3 Automated High-throughput Testing


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◆ Automatic instrument control


● File tree

- MATLAB data analysis
- Oscilloscope video stream
- PC Python Script
- Osc1OCR.py
- LakeShore Model 335
- LakeShore M335.py
- Keithley 2450/2400
- Keithley2450_Isweep.py
- SR 400 Photon Counter
- SRS400.py
- Keysight 33500B
- FuncGene.py

● Test platform





HTP platform's instruments are automatically controlled by the Python, could testing of **device electrical transport (source-meter control)**, **photoelectric response (light source and chopper control)**, and **transient response characteristics (oscilloscope and photon counter)**.

Open source here! 

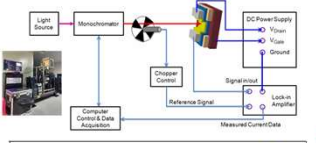
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3 Automated High-throughput Testing

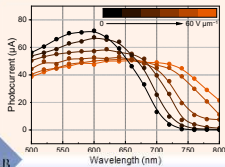



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◆ Transient response and analysis



Q1 Characteristic information of photoelectric response has not been fully mined

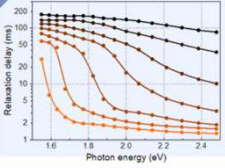


光电响应度光谱特征

Responsivity

- $V_G \uparrow \lambda_{\text{cutoff}} \uparrow$
- $V_G \uparrow \eta_{\text{eqs}} \uparrow$

Consistent with previous



光电弛豫光谱特征



Relaxation

- $V_G \uparrow$ Relax. Time!
- $\lambda \uparrow$ Relax. Time!

New Feature!

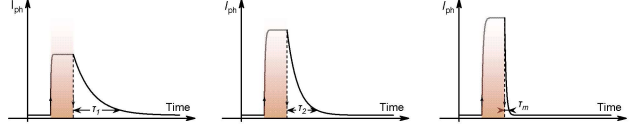
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3 Automated High-throughput Testing

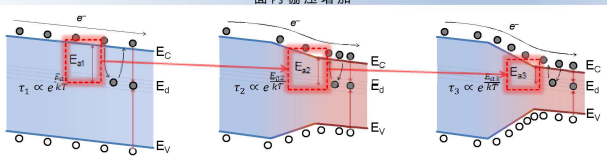



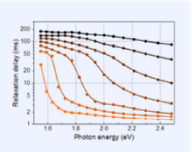
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◆ Carrier kinetic image for relaxation feature



面内栅压增加





Relaxation Feature

Band compression ↓

Shallow defect energy ↓

Boost Recombination ↓



Relaxation time decrease ↓

$$\frac{dn_{\text{free}}}{dt} = k_{\text{light}} n_{\text{trap}} - k_{\text{trap}} n_{\text{free}} \left(1 - \frac{n_{\text{free}}}{N_{\text{trap}}}\right) \quad \frac{dn_{\text{trap}}}{dt} = -k_{\text{non-rad}} n_{\text{trap}} - k_{\text{light}} n_{\text{trap}} + k_{\text{trap}} n_{\text{free}} \left(1 - \frac{n_{\text{free}}}{N_{\text{trap}}}\right)$$

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4 AI Assisted Spectral Reconstruction

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Q1 Characteristic information of photoelectric response has not been fully mined

New Feature !

Q How to introduce relaxation time

$\tau_1 + \tau_2 \neq \tau_3$

$I(\tau_1 + t_0) = A_1 e^{-\frac{t_0}{\tau_1}} = \frac{A_1}{e}$ \Rightarrow $I(\tau_n) = \sum_{i=1}^n A_i e^{-\frac{t_0}{\tau_i}} = \frac{A_n}{e}$

The relaxation time is nonlinear superposition and coupled with responsiveness

Q2 Optimize signal sampling and design reconstruction algorithm is important

The scheme of waveform sampling fitting relaxation time is inefficiency and poor anti-noise

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4 AI Assisted Spectral Reconstruction

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◆ Dual-signal readout method

Relax. time: $\tau \frac{dy}{dt} + y = x$ $\xrightarrow{y(t) = A \sin(\omega t - \phi)}$ $\begin{bmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{bmatrix} \begin{bmatrix} 1 \\ 1/\omega\tau \end{bmatrix} = \begin{bmatrix} 1/k \\ 0 \end{bmatrix}$

Phase difference

Readout Circuit

- ✓ High speed samp.
- ✓ Embedded friendly
- ✓ Time-domain noise controllable
- ✓ Adjustable sampling frame frequency

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4 AI Assisted Spectral Reconstruction

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◆ Artificial neural network reconstruction

ANN Reconstruction

- ✓ Strong nonlinear fitting capability
- ✓ Excellent numerical stability
- ✓ Strong robustness
- ✓ Effective suppression of flicker noise

Q2 Optimize signal sampling and design reconstruction algorithm is important

Sampling ✓ Dual-signal readout circuit

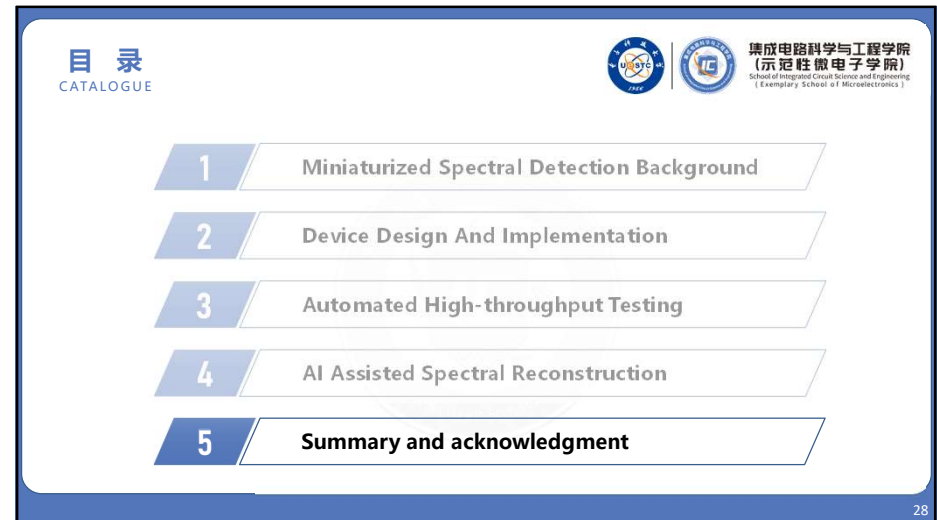
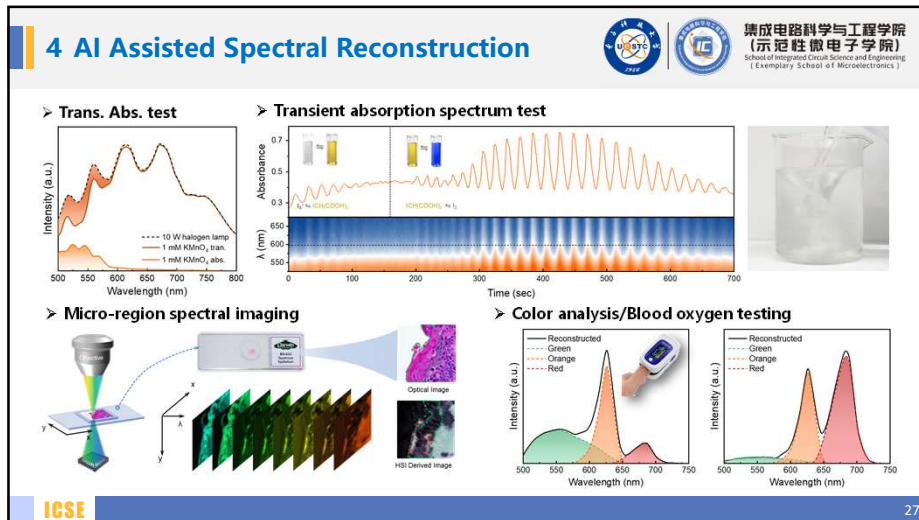
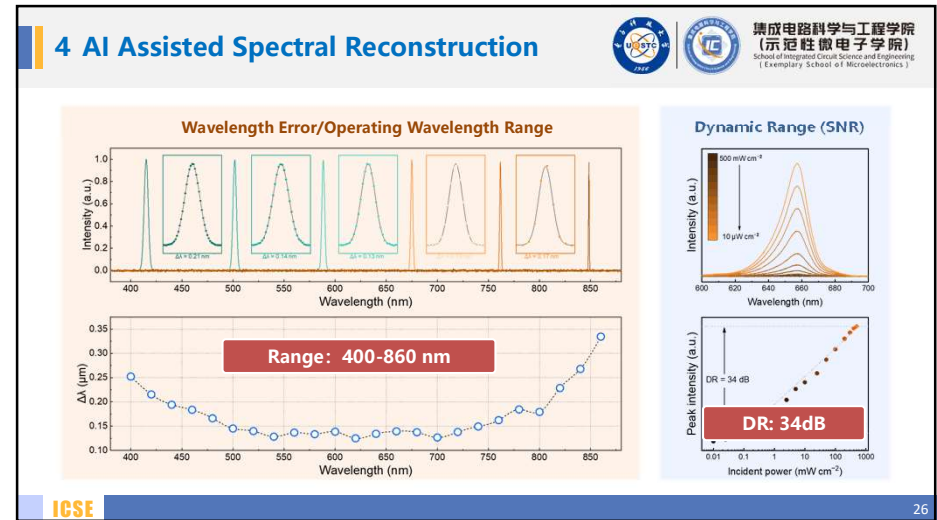
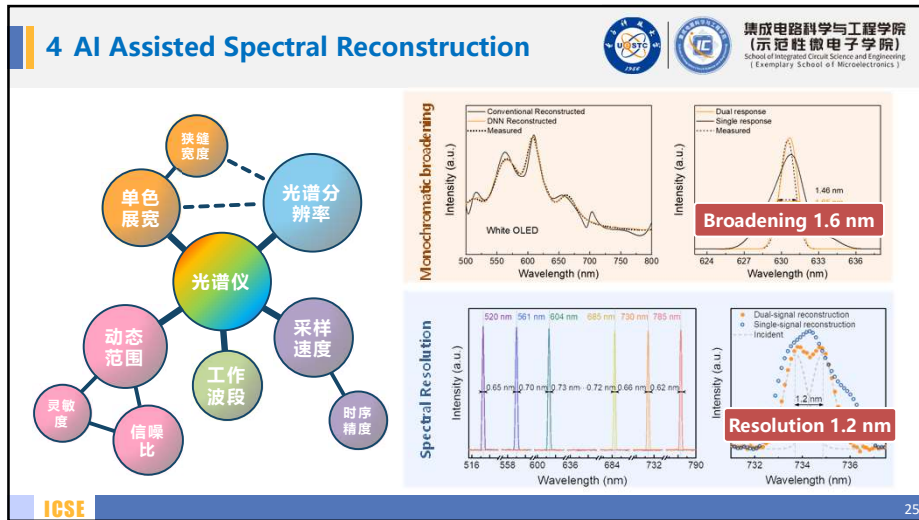
Algorithm ✓ ANN reconstruction algorithm

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4 AI Assisted Spectral Reconstruction

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5 Tech. Prospect

Tech. route perspective: single point spectral detector can effectively **break through the trade-off** between spectral detection volume and accuracy

Legend: Photodetector (red circle), Filter Array (blue triangle), Optical waveguide (grey square).
Nat Electron (2024), 10.1038/s41928-024-01242-9
Sun et al.
Xia et al.

Development process perspective: single point spectral detector can be experiencing **rapid iteration** and **vigorous development** of technology

Legend: Photodetector (red circle), Filter Array (blue triangle), Optical waveguide (grey square).
Nat Electron (2024), 10.1038/s41928-024-01242-9
Our work
Sun et al.
Xia et al.

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5 Summary

Core How to improve **precision** in **S.P. detection**?

Q1 Characteristic information of photoelectric response has not been fully mined

Discover new phenomena

AI HTP Platform

Q2 Optimize signal sampling and design reconstruction algorithm is important

Data deep mining

AI Data Process

Training Sample → Design Optimization

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5 Acknowledgments

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Prof. Zhao Yicheng Prof. Cui Hanxiao Prof. Yang Zongyin PhD Wen Qingsong

Participating students:

Xinchuan Du PhD Yang Wang PhD Yi Cui PhD Ting Zhou Master

Funding Organization:

Laboratory team:

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谢 谢
UESTC

追求卓越 勇创先锋

Basic mechanism




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Basic mechanism




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Basic mechanism



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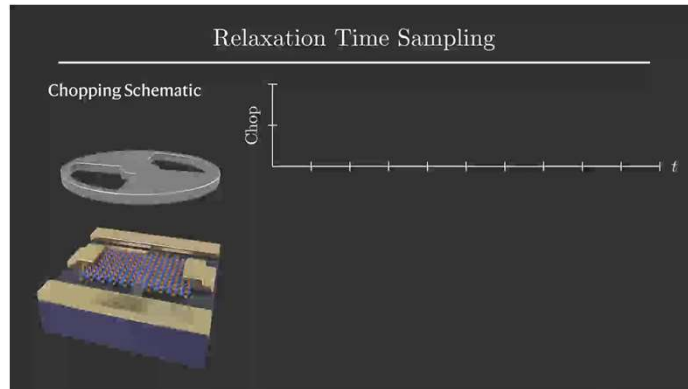
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Relaxation Time Sampling



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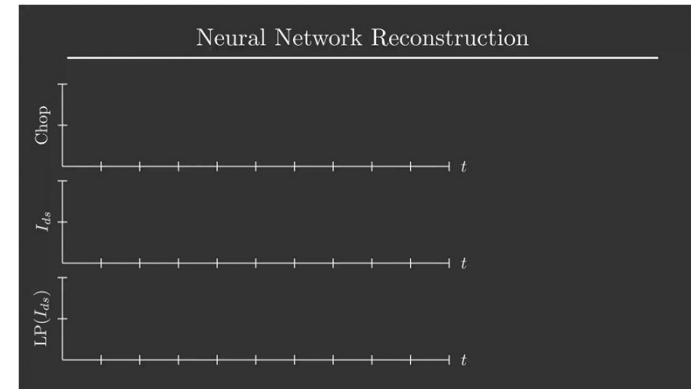
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Neural Network Reconstruction



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