Kosuke Nakago

ENGINEER

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Tokyo, Japan acc1ssnn9terias@gmail.com LinkedIn profile

Kosuke Nakago is an Applied Engineer at Sakana AI. He received his master's degree in physics from the University of Tokyo in 2014. He worked on deep learning research & development at Preferred Networks, Inc. and developed chainer-chemistry, A Library for Deep Learning in Biology and Chemistry. He involved in product launch and release of Matlantis, AI-driven universal high-speed atomistic simulator, and is a launching member of Preferred Computational Chemistry, Inc. He involved in LLM development, leaded instruction tuning part of PLaMo-100B-Instruct at Preferred Elements, Inc. His research interest includes deep learning technology as well as its application to industry. He also participates data science competition, and he is Kaggle competitions grandmaster and notebooks grandmaster.

EXPERIENCE

January 2025 – Present
Applied Engineer, *Sakana AI.*

Started new journey to apply Sakana AI's cutting-edge technology to industry, aiming to deliver real-world value. Currently focusing on AI Agent and related technologies.

March 2024 - December 2024
Engineer, *Preferred Elements, Inc.*

As an Engineering Manager of Alignment team, he leaded instruction tuning part of the GENIAC project to release PLaMo-100B-Instruct model.

July 2021 – Aug 2024
Technical Sales Engineer, *Preferred Computational Chemistry, Inc.*

As a launching member, he contributed to build an organization and workflow for the sales & customer success of Matlantis, universal high-speed atomistic simulator.
Organized to write atomistic simulation tutorial and presented technical background of Matlantis in the seminars worldwide (as listed below) to promote the recent advance of computation-driven materials discovery. Involved in global expansion, consider go-to-market strategy, planning and attending at CES exhibition as marketing etc.

November 2016 – December 2024
Engineer, *Preferred Networks, Inc.*

[Materials Science, Team launches to Matlantis R&D]
Joined 4th IT drug discovery contest (第４回 IT創薬コンテスト), and contributed in winning grand prize

(IPAB賞).
Published OSS chainer-chemistry, which is graph neural network based molecular property prediction library.
Involved in starting materials science & drug discovery team and was an Engineering Manager. Especially, he focused on the collaborative research with ENEOS for the new materials discovery. The research project grows bigger, resulted in releasing SaaS Matlantis, deep learning based atomistic simulator.

[Industry Solutions, Co-Research]
Conducted collaborative research with various Tier 1 company, including manufacturing, automobile, semi-conductor industry. Used various machine learning/deep learning technology and optimization algorithms.

Apr 2014 – Oct 2016
Software Engineer, *Sony EMCS (Malaysia) Sdn Bhd.*

Implemented picture quality driver for Sony's worldwide TV, written in C language. Communicated with the vendor to manage the project.
Implemented prototype of Android TV app, web app for ASEAN region. Used JAVA, javascript, React etc. Going business trip worldwide for the product presentation support & mass manufacturing pipeline launch support.

EDUCATION

Apr 2012 – Mar 2014
Master degree, Physics, The University of Tokyo

Apr 2008 – Mar 2012
Bachelor degree, Applied Physics, Waseda University

SEMINARS

- 第55回 IBISML研究会 2024/12/20
  - Event page, Speakerdeck
- LLM.jp 第13回LLM勉強会 2024/10/29
  - Event page, Twitter, Slide
- Rist Meetup 2024「Kaggleは業務の役にたつ」 2024/10/12
  - Event page, Speakerdeck, Twitter
- CECAM "Perspectives and challenges of future HPC installations for atomistic and molecular simulations" 2024/2/21
  - Event page, Blog, Speakerdeck
- Committee for the Creation of AI-based Systems (AI活用型システム創成委員会 第10回研究会) 2023/10/18
  - "PFNにおける生成AIとシステム"
  - Event page

- MRS Webinar 2023/10/4
  - “History towards Universal Neural Network Potential for Material Discovery”
  - Event page, Video archive, Blog, SpeakerDeck
- QPARC 2022/11/11
  - “スタートアップが提案する2030年の材料開発”
  - Slideshare
- POL 2022/4/22
  - “PFP：材料探索のための汎用Neural Network Potential”
  - Event page, Slideshare, YouTube
- QPARC 2021/12/14
  - “PFP：材料探索のための汎用Neural Network Potential”
  - Slideshare, Twitter
- QCMSR 2021/11/4
  - “PFP：材料探索のための汎用Neural Network Potential”
  - Slideshare, Twitter
- Chemical Society of Japan Keynote Speech (日本化学会 基調講演) 2021/3/21
  - “Deep learningの発展と化学反応への応用”
  - Program, Slideshare
- Kaggle Lyft Motion Prediction for Autonomous Vehicles Webinar 2021/1/26
  - "Forth place winning solution summary"
  - Event page
- IIBMP2019（日本バイオインフォマティクス学会2019年年会 第8回生命医薬情報学連合大会）
  - “オープンソースで始める深層学習”
  - Slideshare (My presentation part p52~p81)
- DLLAB：異常検知ナイトでの講演 @ マイクロソフト
  - “異常検知ハンズオン”
  - Event page, Blog, Slideshare
- Chainer Chemistry seminar (田之倉先生主催の構造生物研究会 - Chainer Chemistry講演 東京大学)
  - “Introduction to Chainer Chemistry”
  - Slideshare

MEDIA INTERVIEWS

- 【PR】汎用原子レベルシミュレータMatlantis™ を提供するPFCC事業開始から1年　DXによって広がる材料探索の可能性 | 日本の研究.com

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OSS & TUTORIALS

- Android TV App Turorial – blog, github
- Deep learning tutorial with Chainer – blog, github
- chainer-chemistry - github
- torch-dftd - github
- Atomistic simulation tutorial – docs, github

KAGGLE ACTIVITIES

He participates various competitions hosted on Kaggle to learn new technologies in various domains.

- Competition achievements
  - 2023 Nov: Kaggle LLM Science Exam 5th place (prize winner, team gold)
    - The task is to answer difficult science questions using LLMs, where the question is generated from Wikipedia data source.
    - Keyword: LLM, Retrieval Augmented Generation (RAG)
  - 2021 May: Human Protein Atlas - Single Cell Classification 7th place (team gold)
    - The task is to classify cell from microscope images.
    - Keyword: CNN, Bio image
  - 2020 Nov: Lyft Motion Prediction for Autonomous Vehicles 4th place (prize winner, team gold)
    - The task is to predict vehicle's future motion in 3 possible trajectories with their probabilities from the bird-view image.
    - Keyword: CNN, Uncertainty prediction
  - 2019 Jun: LANL Earthquake Prediction 19th place (team gold)
    - The task is to predict upcoming laboratory earthquakes, given 1d time-series sensor data.
    - Keyword: CNN, GBDT, sensor data, signal processing
  - 2019 Mar: PetFinder.my Adoption Prediction 13th place (solo gold)
    - The task is to predict how quickly the pet is adopted, given photos, description texts and some metadata of dogs/cats.
    - Keyword: Multi-modal (image, text, features), ranking system, Neural Network, GBDT
  - Based on these achievements, he became **Kaggle Competitions Grandmaster** on 2023 Nov.
- Notebooks
  - Contributed to the activation of Kaggle community by sharing his ideas/findings through the notebooks and became **first Japanese Kaggle Notebooks Grandmaster** on 2021 Feb.
  - Refer below link for the list of notebooks.
  - https://www.kaggle.com/corochann/notebooks?userId=518134&sortBy=voteCount

PUBLICATIONS

1. Kenshin Abe, Kaizaburo Chubachi, Yasuhiro Fujita, Yuta Hirokawa, Kentaro Imajo, Toshiki Kataoka, Hiroyoshi Komatsu, Hiroaki Mikami, Tsuguo Mogami, Shogo Murai, **Kosuke Nakago**, Daisuke Nishino, Toru Ogawa, Daisuke Okanohara, Yoshihiko Ozaki, Shotaro Sano, Shuji Suzuki, Tianqi Xu, Toshihiko Yanase. "PLaMo-100B: A Ground-Up Language Model Designed for Japanese Proficiency". arXiv: 2410.07563 (2024)
2. Ryohto Sawada, **Kosuke Nakago**, Chikashi Shinagawa, So Takamoto. "High-throughput investigation of stability and Li diffusion of doped solid electrolytes via neural network potential without configurational knowledge". Scientific Reports (2024)
3. Dr. Akira Ohno, Prof. Dr. Jun-ichi Hanna, Prof. Dr. Hiroaki Iino, **Kosuke Nakago**, Taiki Yamaguchi, Motoki Abe, Hirotaka Akita, Dr. Mizuki Takemoto. "Universally Exhaustive Generation of Molecular Structures and Prediction of Their Electronic States Using Machine Learning for N-type Organic Transistor Materials". Chemistry An Asian Journal (2023)
4. So Takamoto, Chikashi Shinagawa, Daisuke Motoki, **Kosuke Nakago**, Wenwen Li, Iori Kurata, Taku

Watanabe, Yoshihiro Yayama, Hiroki Iriguchi, Yusuke Asano, Tasuku Onodera, Takafumi Ishii, Takao Kudo, Hideki Ono, Ryohto Sawada, Ryuichiro Ishitani, Marc Ong, Taiki Yamaguchi, Toshiki Kataoka, Akihide Hayashi, Nontawat Charoenphakdee & Takeshi Ibuka "Towards universal neural network potential for material discovery applicable to arbitrary combination of 45 elements". Nature comm 2991 (2022)
The paper is selected as **editor's highlights on 2 categories**; "AI and machine learning" & "Materials science and chemistry".

5. Gerardo Valadez Huerta, Yusuke Nanba, Iori Kurata, **Kosuke Nakago**, So Takamoto, Chikashi Shinagawa, Michihisa Koyama. "Calculations of Real-System Nanoparticles Using Universal Neural Network Potential PFP". arXiv:2107.00963 (2021)
6. Kaushalya Madhawa, Katushiko Ishiguro, **Kosuke Nakago**, Motoki Abe. "GraphNVP: An Invertible Flow Model for Generating Molecular Graphs". arXiv:1905.11600 (2019)
7. Hirotaka Akita, **Kosuke Nakago**, Tomoki Komatsu, Yohei Sugawara, Shin-ichi Maeda, Yukino Baba, Hisashi Kashima. "BayesGrad: Explaining Predictions of Graph Convolutional Networks". arXiv:1807.01985 (2018)
8. **Kosuke Nakago**, Michal Hajdušek, Shojun Nakayama, Mio Murao. "Parallelizable adiabatic gate teleportation". Phys. Rev. A 92, 062316 (2015)

SKILLS

Software: Python, Android/Android TV, C/C++, JAVA, Web (HTML, CSS, javascript, node.js+react etc).
Languages: Native in Japanese, Professional working proficiency in English.

SOCIAL LINKS

- Personal webpage: https://corochann.com
- LinkedIn: https://www.linkedin.com/in/kosuke-nakago-42ba4065/
- Github: https://github.com/corochann
- X (Twitter): https://twitter.com/corochann
- Kaggle: https://www.kaggle.com/corochann
- ORCID: https://orcid.org/0000-0002-8825-4181
- Google Scholar: https://scholar.google.com/citations?user=jqjGH5MAAAAJ