

DƯÁN:

KHÁM PHÁ CÁC VẬT LIỆU CHỨC NĂNG MỚI BẰNG TIẾP CẬN HỌC MÁY **NOVEL FUNCTIONAL MATERIALS DISCOVERY BY MACHINE-LEARNING APP**

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MÃSÔ

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TÓM TẮT VỀ DỰ ÁN

Long-term plan: introduce a new highly-interdisciplinary research area, Materials Informatics, a sub-field of Materials Science and Engineering based on Artificial Intelligence and learning Big Data by computer algorithms, to Vietnamese scientist community.

Immediate goals

- Carry out high-quality research in materials discovery and learning materials data.
- Develop a database of at least 10,000 functional materials structures and accompanied properties, and make it freely available.
- Further contribute to the community by training students, organizing seminars and tutorials in materials informatics, and collaborating with other scientists in Vietnam if common interest is found.
- Develop and maintain a research thrust in Materials Informatics within the PI's group, motivating other Vietnamese groups to involve in this highly-interdisciplinary field.
- Three lines of activities, including (1) materials discovery by structure prediction methods, (2) data curation, taking inputs from line 1 and other sources, and (3) learning the obtained data for structure-properties relations and design rules

THÔNG TIN NỔI BẬT VỀ DỰ ÁN

Công bố 06 bài báo quốc tế (05 SJR Q1, 01 SJR Q2):

(1) V.N. Tuoc, T.D. Huan, Lead-free hybrid organic-inorganic perovskites for solar cell applications, J. Chem. Phys. 152, 014104 (2020) SJR **Q1**, Impact factor: **4.3**

(2) S. Yazdani, V.N. Tuoc , R.K. Sadabad, M.D. Morales-Acosta, Huan T.D., M. Zhou, Y. Liu , J. He, R.D. Montaño, M.T. Pettes, Thermal transport in phase-stabilized lithium zirconate phosphates Appl. Phys. Lett. 117, 011903 (2020) SJR Q1, Impact factor: **3.97**

(3) V.N.Tuoc, N.T. Thao, L.T.H. Lien, P.T. Liem 'Novel Chain and Ribbon ZnO Nanoporous Crystalline Phases in Cubic Lattice. Phys. Stat. Solidi B, 2100067 (2021) 0370-1972, SJR Q2, Impact factor: **1.86**

(4) Minh T. P, E. Amerling, Anh. T. Ngo, Hoang M. Luong, K. Hansen, Huy T. P., Tuoc N. Vu, Huan Tran, L. Whittaker-Brooks, and Tho D. Nguyen Strong Rashba-Dresselhaus Effect in Non-chiral 2D Ruddlesden-Popper Perovskites, 2021 Adv. Optical Mater. 2021, 2101232, SJR **Q1**, Impact factor: **9.93**

(5) V.N. Tuoc, Nga T. T. Nguyen, V. Sharma, and T.D. Huan, Probabilistic deep learning approach for targeted hybrid organic-inorganic perovskites, Physical Review Materials, 5, 125402 (2021)SJR Q1, Impact factor: 3.98

(6) T.D. Huan, V.N. Tuoc, Machine-learning approach for discovery of conventional superconductors, Physical Review Materials, 7, 054805 (2023), SJR **Q1**, Impact factor: **3.98**

Bộ cơ sở dữ liệu cấu trúc: Năm 2020 là http://www.godeepdata.org/ và từ 2021 chuyển sang host mới là

http://matsml.org/index_files/data.html (bao gồm 07 data set ~ 10k cấu trúc) **Bộ công cụ:** Bộ công cụ phần mềm để nghiên cứu vật liệu bằng phương pháp học máy - Machine learning toolkit for

materials science (MATSML) được chia xẻ miến phí cho cộng đồng htts://github.com/huantd/matsml Hội thảo quốc tê: 03 nternational Symposium on Materials Informatics 2020 hosted by Japan Advanced Institute of Science and Technology (JAIST); Joint 5th International Symposium on Frontiers in Materials Science & 3rd Interna-tional Symposium on Nano-materials, Technology and Applications (FMS-NANOMATA 2019) and (FMS-2022).

Đào tạo: 01 Thạc sỹ Vật lý lý thuyết và Vật lý Toán - đã bảo vệ 6/2021. Giải thưởng:

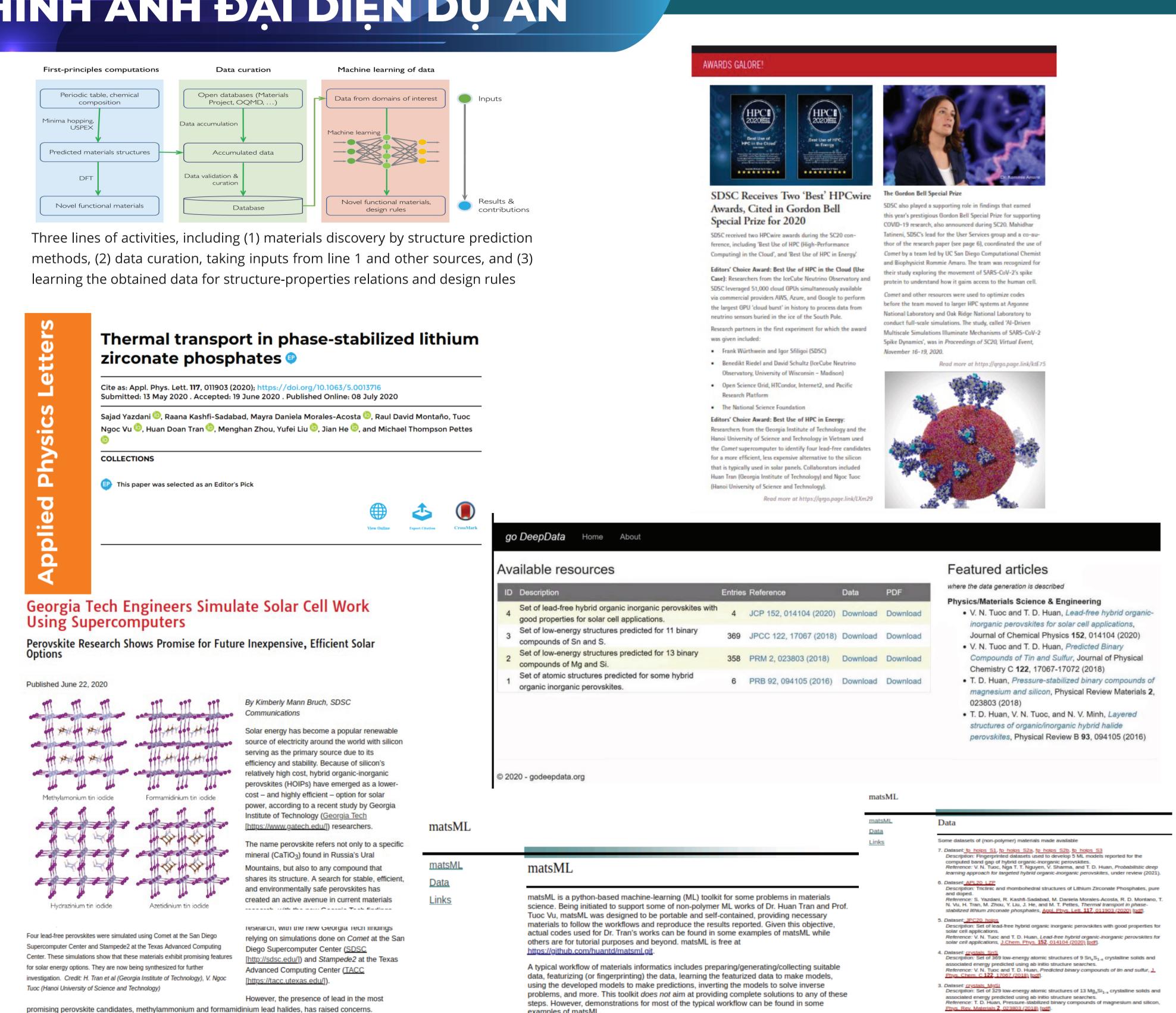
Các cấu trúc mới dự đoán trong (1) đã được đưa tin trên trang của UCSD News [https://ucsdnews.ucsd.edu/pressrelease /georgia-tech-engineers-simulate-solar-cell-work-using-supercomputers].

Công bố (2) được Biên tập của J. Appl. Phys. Lett. chọn là công bố tiêu biểu (Editor's Pick – EP)

[https://aip.scitation.org/doi/abs/10.1063/5.0013716].

Bài báo số 1 được Ban Biên tập của Tạp chí HPC Wire bình chọn cho Giải thưởng "Best Use of HPC in Energy" [link giải thưởng https://www.hpcwire.com/readers-and-editors-choice-awards-2020-winners/; link trao giải https://youtu.be/EnV5cEiFjzA]





Most of the computed data referred to in this toolkit are from Huan Tran and Tuoc Vu's works

(see here), supported by the XSEDE's DMR170031 project; others are open reported data. In

cases of experimental data that are subjected to copyright and ownership, suitable freely

available alternatives are provided for demonstration purpose. Questions, requests, and

comments are welcome at huantd@gmail.com.

Dataset: PRB16 holps
 Description: Set of atomic structures predicted for some hybrid organic inorganic

Description: Each dataset contains 10,000 non-equilibrium (perturbed) atomic configurations (of either of CH₄ or CH₃-NH-OH molecule) and associated ener

computed using <u>BigDFT</u> and norm-conserving HGH pseudopotentials. Reference: Huan Tran, unpublished.

perovskites. Reference: T. D. Huan, V. N. Tuoc, and N. V. Minh, Layered structures of organic/inorganic

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Moreover, these materials have shown to be unstable under certain environmental conditions.

The Georgia Tech researchers worked with colleagues at the Hanoi University of Science and Technology in

Vietnam to create simulations that identified four lead-free perovskites as promising candidates for solar cell

materials. Two of them have already been synthesized and the other two are recommended for further