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Keywords: DFT-based machine learning, Machine Learning Force Field, predicting material properties.

Summary of research: Machine learning force fields (MLFF) that incorporate density functional theory (DFT) data can significantly reduce the computing time, making it more feasible to explore a wider range of materials and properties. By training on DFT-based data, MLFF can capture complex quantum mechanical interactions that are essential for accurately predicting material properties. Several of the material properties that can be suitable in prediction using MLFFs, for example, structural properties, elastic properties, thermodynamic properties, thermal properties. phonon dispersion, molecular adsorption, and catalytic activity. The predicting material properties by machine learning is beneficial to guide experimentalists in reducing the trial-and-error aspect of materials development.

แบบเสนอโครงการวิจัย (Research Project)
ประกอบการเสนอขอทุนอุดหนุนการวิจัยของสำนักงานการวิจัยแห่งชาติ (วช.)
โครงการปริญญาเอกกาญจนาภิเษก (คปก.) ภายใต้ความร่วมมือไตรภาคีไทย-สวีเดน
ประจำปีงบประมาณ ๒๕๖๗

๑. **ชื่อโครงการวิจัย**

DFT-based machine learning force field for materials informatics

๒. **ชื่อ-สกุล อาจารย์ที่ปรึกษา**

Assoc. Prof. Adisak Boonchun, Ph.D. (รศ.ดร.อดิศักดิ์ บุญชื่น)
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๓. **กลุ่มสาขาวิทยาศาสตร์พื้นฐานที่สมัคร** (เลือกเพียง ๑ กลุ่ม)

☐ ชีววิทยา (Biology) ☐ เคมี (Chemistry)
☑ ฟิสิกส์ (Physics) ☐ คณิตศาสตร์ (Mathematics)

๔. **ผู้ใช้ประโยชน์ (Research stakeholders)** (กรณีมีความร่วมมือฯ) เช่น ความร่วมมือของหน่วยงานภาครัฐ (เช่น กระทรวง กรม)/เอกชนที่ร่วมสนับสนุนทุนวิจัย เช่น MOU เป็นต้น

☐ มี.....*(โปรดระบุชื่อความร่วมมือ และหน่วยงาน)*.....
☑ ไม่มี

๕. **คำสำคัญ (Keyword) ของโครงการ**

DFT-based machine learning, Machine Learning Force Field, predicting material properties.

๖. **ความสำคัญและที่มาของปัญหาที่ทำการวิจัย (Problem statement and significance of research)**

Density Functional Theory (DFT) is a widely used quantum mechanical method to study materials at the atomic scale. However, DFT calculations can be computationally expensive, especially for large and complex systems. Machine learning force fields (MLFF) that incorporate DFT data can significantly reduce the computational cost, making it more feasible to explore a wider range of materials and properties. By training on DFT-based data, MLFF can capture complex quantum mechanical interactions that are essential for accurately predicting material properties. This level of accuracy is crucial for guiding experimental efforts and reducing the trial-and-error aspect of materials development.

๗. **ทฤษฎี/สมมุติฐานของโครงการ (Hypothesis)**

The theory of DFT-based machine learning force fields combines concepts from DFT and machine learning algorithms to develop efficient and accurate models for predicting the potential energy surface of materials. The main idea is to learn the potential energy surface (PES) of a material from a limited set of DFT data and then use this learned information to predict the energy and other properties of the material at new, unexplored configurations.

The potential energy surface of a material in DFT is given by the electronic energy, which depends on the positions of all atoms in the system. In a machine learning force field, the potential energy surface is typically represented as a sum of atomic contributions:

$$E(\boldsymbol{R}) = \sum_{i} E_{atom}(\boldsymbol{R}_i)$$

where $E(\boldsymbol{R})$ is the total potential energy of the system with atomic positions $\boldsymbol{R}$, and $\sum_{\{i\}} E_{atom}(\boldsymbol{R}_i)$ is the energy contribution from atom i at position $\boldsymbol{R}_i$.

The key idea behind the machine learning component is to approximate these atomic energy contributions using a machine learning model, such as neural networks, kernel ridge regression, or Gaussian processes. The model is trained on a dataset of DFT-calculated energies and corresponding atomic configurations.

Once the machine learning force field is trained, it can be used to predict the energy and other properties of materials for a wide range of atomic configurations, even ones that are computationally infeasible to calculate using DFT directly.

๘. **วัตถุประสงค์ของโครงการ (Objectives)**

The objective of this research is to use DFT-based on-the-fly machine learning force fields predict material properties efficiently and accurately.

๙. **การทบทวนวรรณกรรม/ผลงานวิจัยที่เกี่ยวข้อง (Literature Review)**

The concept of "DFT-based on-the-fly machine learning force fields" using the VASP (Vienna Ab Initio Simulation Package) code was an introduced in 2020. Below are some literature reviews of relevant papers that discuss and application on active machine learning force field:

1. Jinnouchi, R., Karsai, F., & Kresse, G. (2019). *On-the-fly machine learning force field generation: Application to melting points*. Physical Review B, 100(1), 014105. This paper

present an efficient on-the-fly machine learning force field that can be applied to liquid-solid phase transitions of Al, Si, Ge, Sn and MgO.

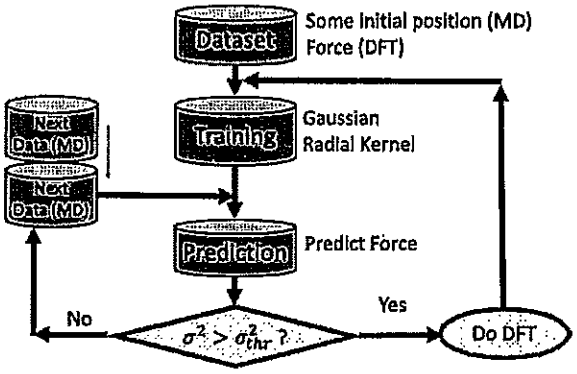
2. Jinnouchi, R., Lahnsteiner, J., Karsai, F., Kresse, G., & Bokdam, M. (2019). *Phase transitions of hybrid perovskites simulated by machine-learning force fields trained on the fly with Bayesian inference*. Physical review letters, 122(22), 225701.
3. Jinnouchi, R., Miwa, K., Karsai, F., Kresse, G., & Asahi, R. (2020). *On-the-fly active learning of interatomic potentials for large-scale atomistic simulations.* The Journal of Physical Chemistry Letters, 11(17), 6946. The authors present three applications: catalytic activity of alloyed nanoparticles (NPs), entropy-driven phase transitions of hybrid perovskites, and nuclear quantum effects on thermodynamics and kinetics of an AB_2-type Laves hydride.

๑๐. ระเบียบวิธีวิจัย (Methodology)

Here's a outline of the on-the-fly MLFF methodology steps:

1. Data Generation and Feature Engineering
   - Perform MD simulation to obtain a dataset of atomic configurations ($\boldsymbol{R}$) and perform DFT at a dataset of $\boldsymbol{R}$ to obtain the corresponding potential energies ($\boldsymbol{E}$).
   - Convert atomic configurations ($\boldsymbol{R}$) into feature vectors ($\boldsymbol{X}$) by using descriptors.
3. Model Training:
   - Use the feature vectors ($\boldsymbol{X}$) and corresponding potential energies ($\boldsymbol{E}$) to train a machine learning model.
4. On-the-Fly Prediction:
   - During molecular simulations, use the trained machine learning model to predict potential energies on-the-fly for each new atomic configuration encountered.
5. Accuracy Assessment and Iterative:
   - Calculate the Bayesian error. If the error is high, DFT calculations will be performed. If the error is low, the new atomic configuration from the next step of molecular dynamics will be used as reiterate input.

Here's a flowchart of the on-the-fly MLFF steps:



๑๑. ขอบเขตของการวิจัย (Scope of the study)

The scope of the study of this proposal is to use DFT-based on-the-fly machine learning force fields, implemented in VASP code, develop for predicting material properties. Some of the material properties that we are interested in prediction using MLFFs include: structural properties, elastic properties, phonon dispersion, molecular adsorption and thermal properties.

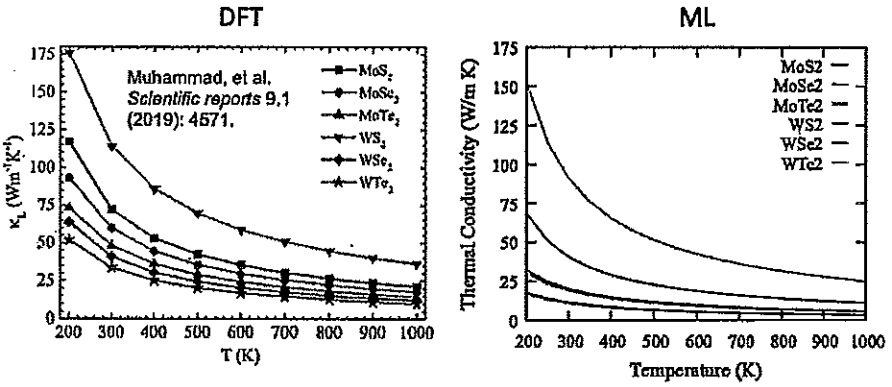
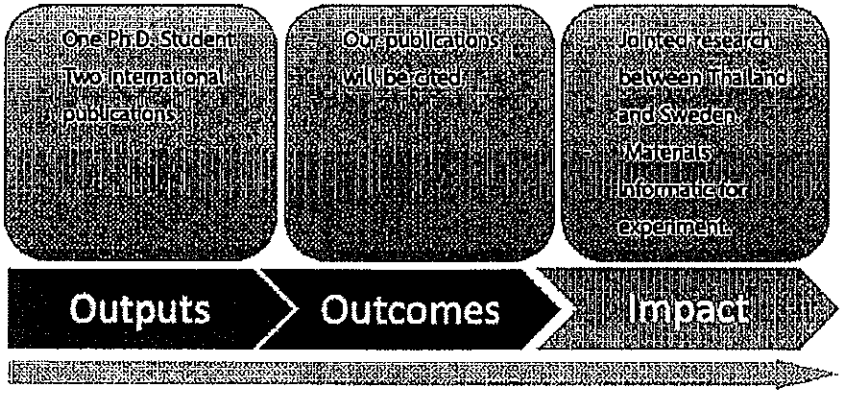


Fig. 1 An example: Thermal conductivity of Transition-Metal Dichalcogenides (TMDs) by using (a) DFT and (b) on-the-fly MLFF method (Fig.1(b) is our unpublished work)

๑๒. ผลผลิต (Output) ผลลัพธ์ (Outcome) และ ผลกระทบ (Impact) ที่คาดว่าจะได้จากการวิจัย



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ABOUT ME

Adisak Boonchun received his Ph.D. degree at Case Western Reserve University at Department of Physics in 2011. A. Boonchun was conducting his research under supervision of Prof. Walter Lambrecht focus on optical transitions, vibrations, cohesive and elastic properties in wide-band gap semiconductor. In 2011, he had a first taste of a postdoc in National Institute for materials science (NIMS) in Japan. In 2013, he joined the department of physics, Kasetsart University and was promoted to assistant professor in 2016. His research interests focus on electronic and mechanic properties of 2D materials and intercalation voltage in novel Li-ion battery.

EXPERIENCE

Associate Professor in Physics
Kasetsart University
Dec 2019 – Ongoing Bangkok, TH

Assistant Professor in Physics
Kasetsart University
Dec 2016 – Dec 2019 Bangkok, TH

Lecturer in Physics
Kasetsart University
Sep 2013 – Dec 2016 Bangkok, TH

Postdoctoral Fellows
National Institute for materials science (NIMS), Japan
Oct 2011 – Sep 2013 Tsukuba, JP

Research Assistant
CWRU
2007 – 2011 Cleveland, Ohio, US

LICENSES & CERTIFICATIONS

Complete Tensorflow 2 and Keras Deep Learning Bootcamp
Jan 2021 Udemy

Programming Numerical Methods in Python
Jan 2021 Udemy

Data Visualization with Python for Beginners
Jan 2021 Udemy

EDUCATION

Ph.D. in Physics
Case Western Reserve University
Sept Aug 2006 – Aug 2011

M.S. in Physics
Kasetsart University
June 2002 – May 2005

B.S. in Physics
Kasetsart University
June 1998 – May 2002

MOST PROUD OF

Award
Second prize of Thailand's Outstanding Thesis Award from Office of National Research Council of Thailand

Scholarship
Higher Educational Strategic Scholarships for Frontier Research Net- work of Thailand

Scholarship
Development and Promotion of Science and Technology Talents project (DPST) Full Scholarship, Thailand

STRENGTHS

VASP | Abinit & Quantum Espresso | Python & Linux

LANGUAGES

Thai ●●●●●
English ●●●○○

LIFE PHILOSOPHY

"I don't think inside the box,
I don't think outside the box...
I don't even know where the box is."

PUBLICATIONS

Book Chapter

- Boonchun, Adisak (2011). *First-Principles Calculation of Defect Energies in ZnO and Related Materials.*

Journal Articles

- Ananchuensook, Aroon et al. (2023). "Effects of oxygen pressure on the morphology and surface energetics of β-PbO_2: insight from DFT calculations". In: *Physical Chemistry Chemical Physics.*
- Dabsamut, Klichchupong et al. (2023a). "Surface alloy with sulfur leading piezoelectricity from non-piezoelectricity of pentagonal-PdPSe". In: *Journal of Alloys and Compounds* 947, p. 169640.
- Dabsamut, Klichchupong et al. (2023b). "Theoretically proposed stable polymorph of two-dimensional pentagonal β-PdPSe". In: *Physical Chemistry Chemical Physics.*
- Detrattanawichai, Panyalak et al. (2023). "Exploring the impact of the nitrogen layer on a Cu (001) substrate on the spin crossover properties of [Fe (SalEen-I)$_2$] Br: A DFT study". In: *Journal of Physics and Chemistry of Solids* 173, p. 111111.
- Thanasarnsurapong, Thanasee et al. (2023a). "Enabling enhanced lithium storage capacity of two-dimensional pentagonal BN_2 by aluminum doping". In: *Journal of Materials Chemistry C.*
- Thanasarnsurapong, Thanasee et al. (2023b). "Ternary pentagonal BXN (X= C, Si, Ge, and Sn) sheets with high piezoelectricity". In: *RSC advances* 13.14, pp. 9636–9641.
- Worakajit, Pimpisut et al. (2023). "Origin of Hole-Trapping States in Solution-Processed Copper (I) Thiocyanate and Defect-Healing by I_2 Doping". In: *Advanced Functional Materials*, p. 2209504.
- Ananchuensook, Aroon et al. (2022). "Towards a new packing pattern of Li adsorption in two-dimensional pentagonal BCN". in: *Physical Chemistry Chemical Physics* 24.21, pp. 13194–13200.
- Dabsamut, Klichchupong, Adisak Boonchun, and Walter RL Lambrecht (2022a). "Calculated electron paramagnetic resonance g tensor and hyperfine parameters for zinc vacancy and N related defects in ZnO". in: *Physical Review Materials* 6.10, p. 104609.
- – (2022b). "N_2, NO, and O_2 molecules in $LiGaO_2$ in both Ga and Li sites and their relation to the vacancies". In: *Journal of Applied Physics* 131.14, p. 145705.
- Dabsamut, Klichchupong et al. (2022a). "Electric field- and strain-induced bandgap modulation in bilayer C_2N". in: *Applied Physics Letters* 120.20, p. 203101.
- Dabsamut, Klichchupong et al. (2022b). "Two-Dimensional Penta-NiPS Sheets: Two Stable Polymorphs". In: *The Journal of Physical Chemistry C* 126.45, pp. 19455–19461.
- Sukharom, Siwakorn et al. (2022). "Effect of native point defects on the photocatalytic performance of $ZnIn_2S_4$". In: *Physica B: Condensed Matter*, p. 413674.
- Dabsamut, Klichchupong et al. (2021). "Strain engineering and thermal conductivity of a penta-BCN monolayer: a computational study". In: *Journal of Physics D: Applied Physics.*
- Palakawong, Nirawith et al. (2021). "Hybrid-Functional Study of Native Point Defects and Ti/Fe Impurities in α-Al_2O_3". In: *physica status solidi (b)* 258.4, p. 2000498.
- Promchana, Pratya et al. (2021). "Direct conversion of carboxylic acid to olefins over Pt-loaded, oxygen-deficient alkali hexatitanate catalysts with ketonization-hydrogenation-dehydration activity". In: *Catalysis Today* 375, pp. 418–428.

REFEREES

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- Thanasarnsurapong, Thanasee et al. (2021). "Piezoelectric and electronic properties of hydrogenated penta-BCN: A computational study". In: *Journal of Applied Physics* 129.9, p. 095101.
- Charoenphon, Supparat et al. (2020). "Energetics and optical properties of carbon impurities in rutile TiO_2". In: *RSC Advances* 10.33, pp. 19648–19654.
- Dabsamut, Klichchupong, Adisak Boonchun, and Walter RL Lambrecht (2020). "First-principles study of n-and p-type doping opportunities in $LiGaO_2$". In: *Journal of Physics D: Applied Physics* 53.27, p. 274002.
- Promchana, Pratya et al. (2020). "Direct conversion of carboxylic acid to olefins over Pt-loaded, oxygen-deficient alkali hexatitanate catalysts with ketonization-hydrogenation-dehydration activity". In: *Catalysis Today*.
- Skachkov, Dmitry et al. (2020). "Computational study of electron paramagnetic resonance spectra for Li and Ga vacancies in $LiGaO_2$". In: *Journal of Physics D: Applied Physics* 53.17, 17LT01.
- Boonchun, Adisak, Klichchupong Dabsamut, and Walter RL Lambrecht (2019). "First-principles study of point defects in $LiGaO_2$". In: *Journal of Applied Physics* 126.15, p. 155703.
- Dabsamut, Klichchupong et al. (2019). "Stacking stability of C_2N bilayer nanosheet". In: *Scientific Reports* 9.1, p. 6861.
- Pakeetood, Patompob et al. (2019). "Hybrid-functional study of native defects and W/Mo-doped in monoclinic-bismuth vanadate". In: *The Journal of Physical Chemistry C* 123.23, pp. 14508–14516.
- Simalaotao, Kodchakorn et al. (2019). "Energetics of native defects in $ZnRh_2O_4$ spinel from hybrid density functional calculations". In: *Journal of Applied Physics* 125.16, p. 165703.
- Kanchanawarin, Jarin et al. (2018). "Local structure of stoichiometric and oxygen-deficient $A_2Ti_6O_{13}$ (A= Li, Na, and K) studied by X-ray absorption spectroscopy and first-principles calculations". In: *Journal of Applied Physics* 124.15, p. 155101.
- Suwan, Yuwadee et al. (2018). "Structural deformation of nanomembranes in pressurized blister test". In: *Materials Today: Proceedings* 5.5, pp. 11051–11059.
- Jiraroj, T et al. (2017). "Identification of hydrogen defects in α-Al_2O_3 by first-principles local vibration mode calculations". In: *Physical Review B* 95.13, p. 134103.
- Pimsorn, Pimpika et al. (2017). "Reassignment of O-related infrared absorption peaks in CdSe". In: *Ceramics International* 43, S359–S363.
- Boonchun, Adisak, Pakpoom Reunchan, and Naoto Umezawa (2016). "Energetics of native defects in anatase TiO_2: A hybrid density functional study". In: *Physical Chemistry Chemical Physics* 18.43, pp. 30040–30046.
- Reunchan, Pakpoom, Adisak Boonchun, and Naoto Umezawa (2016). "Electronic properties of highly-active Ag_3AsO_4 photocatalyst and its band gap modulation: an insight from hybrid-density functional calculations". In: *Physical Chemistry Chemical Physics* 18.33, pp. 23407–23411.
- Boonchun, Adisak and Walter RL Lambrecht (2013). "Electronic structure of defects and doping in ZnO: Oxygen vacancy and nitrogen doping". In: *physica status solidi (b)* 250.10, pp. 2091–2101.
- Boonchun, Adisak et al. (2013). "Role of photoexcited electrons in hydrogen evolution from platinum co-catalysts loaded on anatase TiO_2: a first-principles study". In: *Journal of Materials Chemistry A* 1.22, pp. 6664–6669.
- Lambrecht, Walter RL and Adisak Boonchun (2013). "Identification of a N-related shallow acceptor and electron paramagnetic resonance center in ZnO: N_2^+ on the Zn site". In: *Physical Review B* 87.19, p. 195207.
- Boonchun, Adisak et al. (2012). "Nitrogen pair- hydrogen complexes in

ZnO and p-type doping." In: *MRS Online Proceedings Library Archive* 1394.

- Boonchun, Adisak and Walter RL Lambrecht (2011a). "Critical evaluation of the LDA+U approach for band gap corrections in point defect calculations: The oxygen vacancy in ZnO case study". In: *physica status solidi (b)* 248.5, pp. 1043–1051.
- Preston, ARH et al. (2011). "First-principles calculation of resonant x-ray emission spectra applied to ZnO". In: *Physical Review B* 83.20, p. 205106.
- Boonchun, Adisak and Walter R. L. Lambrecht (2010a). "First-principles study of oxygen vacancies in $Mg_xZn_{1-x}O$ alloys". In: *Phys. Rev. B* 81 (2), p. 024103.
- Boonchun, Adisak and Walter RL Lambrecht (2010b). "Erratum: First-principles study of the elasticity, piezoelectricity, and vibrational modes in $LiGaO_2$ compared with ZnO and GaN [Phys. Rev. B 81, 235214 (2010)]". In: *Physical Review B* 82.7, p. 079904.
- – (2010c). "First principles study of the elasticity, piezoelectricity, and vibrational modes in $LiGaO_2$ compared with ZnO and GaN". In: *Physical Review B* 81.23, p. 235214.
- Boonchun, Adisak and Walter R. L. Lambrecht (2009). "Bond lengths, phase stability, and band gaps in $Mg_xZn_{1-x}O$ alloys". In: *Journal of Vacuum Science Technology B: Microelectronics and Nanometer Structures Processing, Measurement, and Phenomena* 27.3, pp. 1717–1721.
- Trivijitkasem, Supreya et al. (2009). "Analytical study of AC magnetic susceptibility of (Bi,Pb)Sr-Ca-Cu-O superconducting systems using Bean critical state model". In: *Kasetsart J.(Nat. Sci.)* 43, pp. 353–360.
- Boonchun, Adisak et al. (2007). "First principles study of Mn impurities in $PbTiO_3$ and $PbZrO_3$". In: *Journal of applied physics* 101.4, p. 043521.
- Limpijumnong, Sukit et al. (2007). "Identification of Mn site in $Pb(Zr,Ti)O_3$ by synchrotron x-ray absorption near-edge structure: Theory and experiment". In: *Applied Physics Letters* 90.10, p. 103113.

Conference Proceedings

- Boonchun, Adisak and Walter RL Lambrecht (2011b). "Electronic structure, doping, and lattice dynamics of $LiGaO_2$". In: *Oxide-based Materials and Devices II*. vol. 7940. International Society for Optics and Photonics, 79400N.