Project No. 31006

Report form of Joint Research Project at ZAIKEN (2019)

Title of Project	**Informatics approach for the development of efficient rare-earth free phosphors**		
Priority Area	**Material informatics and environment consciousness**		
New proposal			
Name of Main Applicant	**Nguyen Hai Chau**		
Institution	**Faculty of Information Technology,** **University of Engineering and Technology,** **Vietnam National University**	**title**	**Associate Professor**

Aim of the research project

The aim of this research project is combination of informatics techniques and computational simulations for the construction of databases to develop environmentally conscious materials with demanding properties. At first steps, phosphor is chosen as the target material with long-life, low-cost and high emission intensity as expected properties. During project's early stage, we expanded the target material to high entropy alloys (HEA). The detailed research plan includes the following steps:

1. Automatic first-principles calculations
2. Database construction
3. Prediction of mechanical properties of some HEAs
4. Application of informatics techniques for design of new HEAs
5. Synthesis of the candidate materials

Contents and results of the research

In 2019, we completed steps 1 and 2 by building automatic scripts for first-principles calculations using VASP [1] and for extracting properties of materials from https://materialsproject.org/. For step 3, we used data extracted from work of S. Guo et al [2] and reproduced study of N. Islam et al [3] to predict phases of multi-principal element alloys. Using C5.0 [4] and Random Forests [5] classification methods, we achieved good results in comparison to that of Islam et al. Our mean prediction accuracy using the methods are 82.5% and 86.3%, respectively. Islam et al achieved 83.2% mean accuracy using neural network method [6].
In 2020 we plan to continue the remaining steps of the project starting from prediction of mechanical properties of binary alloys using first-principle calculations and informatics techniques such as deep learning [7].

References

[1] G. Kresse and J. Hafner, *Phys. Rev. B47,* vol. 558, 1993.

[2] S. Guo and C. T. Liu, "Phase stability in high entrpy alloys: Formation of solid-solution phase or amorphous phase," *Progress in Natural Sciences: Materials International,* vol. 21, pp. 433-446, 2011.

[3] N. Islam, W. Huang and H. Zhuang, "Machine learning for phase selection in multi-principal element alloys," *Computational Materials Science,* vol. 150, pp. 230-235, 2018.

[4] J. R. Quinlan, "Improved use of continuous attributes in C4.5," *Journal of Artificial Intelligence Research,* vol. 4, pp. 77-90, 1996.

[5] L. Breiman, "Random forests," *Machine learning,* vol. 45, pp. 5-32, 2001.

[6] W. S. McCulloch and W. Pitts, "A logical calculus of the ideas immanent in nervous activity," *The Bulletin of Mathematical Biophysics,* vol. 5, no. 4, pp. 115-133, 1943.

[7] B. Yoshua, Y. LeCun and G. Hinton, "Deep learning," *Nature,* vol. 521, no. 7553, pp. 436-444, 2015.

Outputs of the project (publications, presentations, patents)

Some of the results will be presented in 2020 at the related international conferences and domestic meetings.