Summit to: Materials Database Construction

Prediction of electron inelastic mean free paths for inorganic compounds with a machine learning approach

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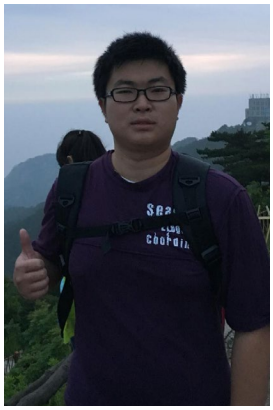
EXTENDED ABSTRACT: Electron inelastic mean free paths (IMFPs) are important parameters in surface analysis methods like electron spectroscopy and microscopy. In previous work[1], we present a machine learning (ML) method using elemental material dependent parameters describe and predict IMFPs of elemental materials from the calculated IMFPs for a group of 41 elemental materials from the paper by Shinotsuka et al.. Based on experience of the prediction of elemental material electron IMFPs, here we continuously extended the usage of the same machine learning method on 42 compounds. Our findings suggest that machine learning is still very efficient and powerful on compounds IMFP description, and possess many advantages than traditional empirical formulae.

Keywords： machine learning; inelastic mean free path

REFERENCES

[1] X. Liu, L.H. Yang, Z.F. Hou, B. Da, K. Nagata, H. Yoshikawa, S. Tanuma, Y. Sun and Z.J. Ding, Phys. Rev. Mater. **5**, 033802 (2021).

[2] X. Liu, Z.F. Hou, D.B. Lu, B. Da, H. Yoshikawa, S. Tanuma, Y. Sun and Z.J. Ding, Sci. Technol. Adv. Mater. **20,** 1090 (2019).



BIOGRAPHY

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