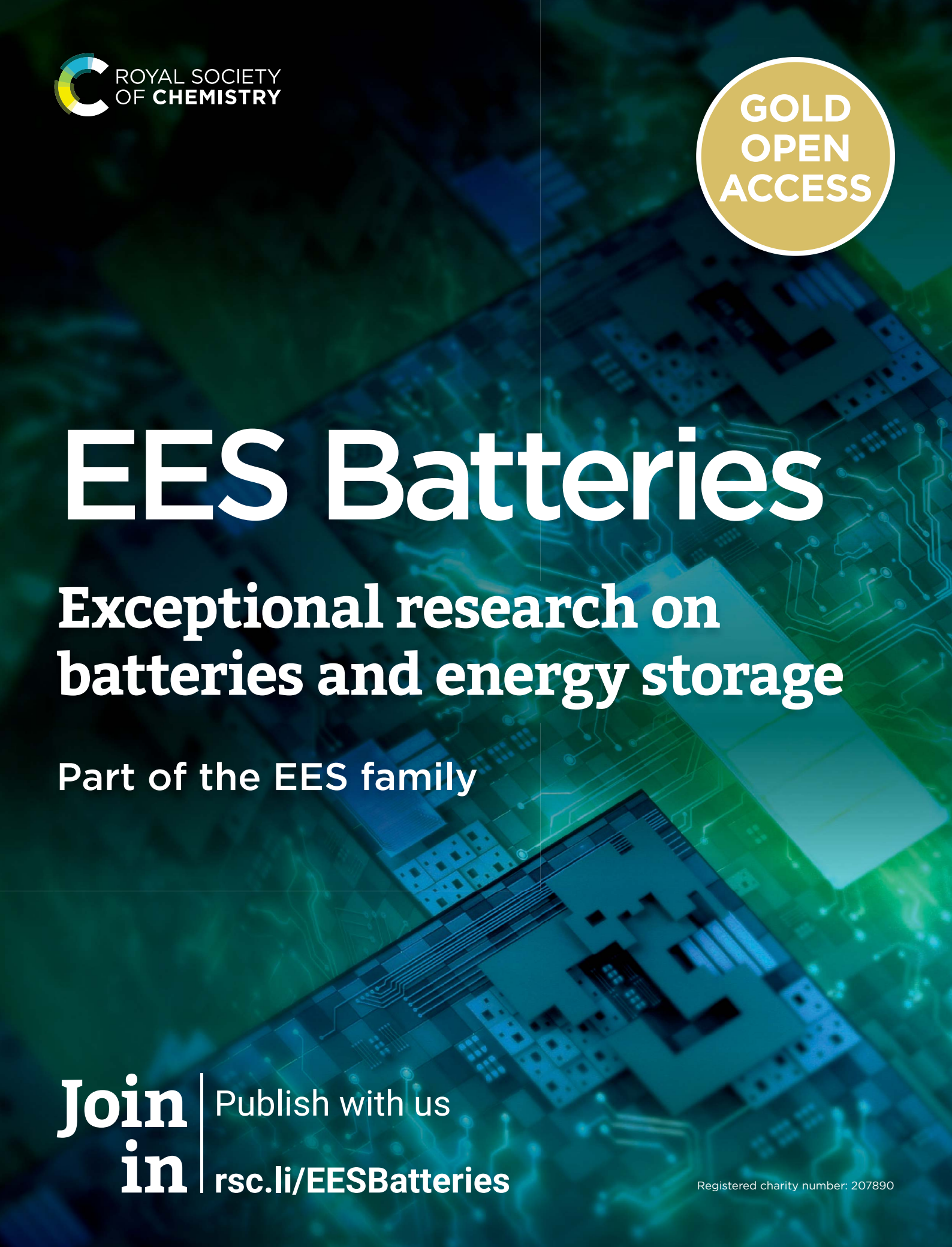
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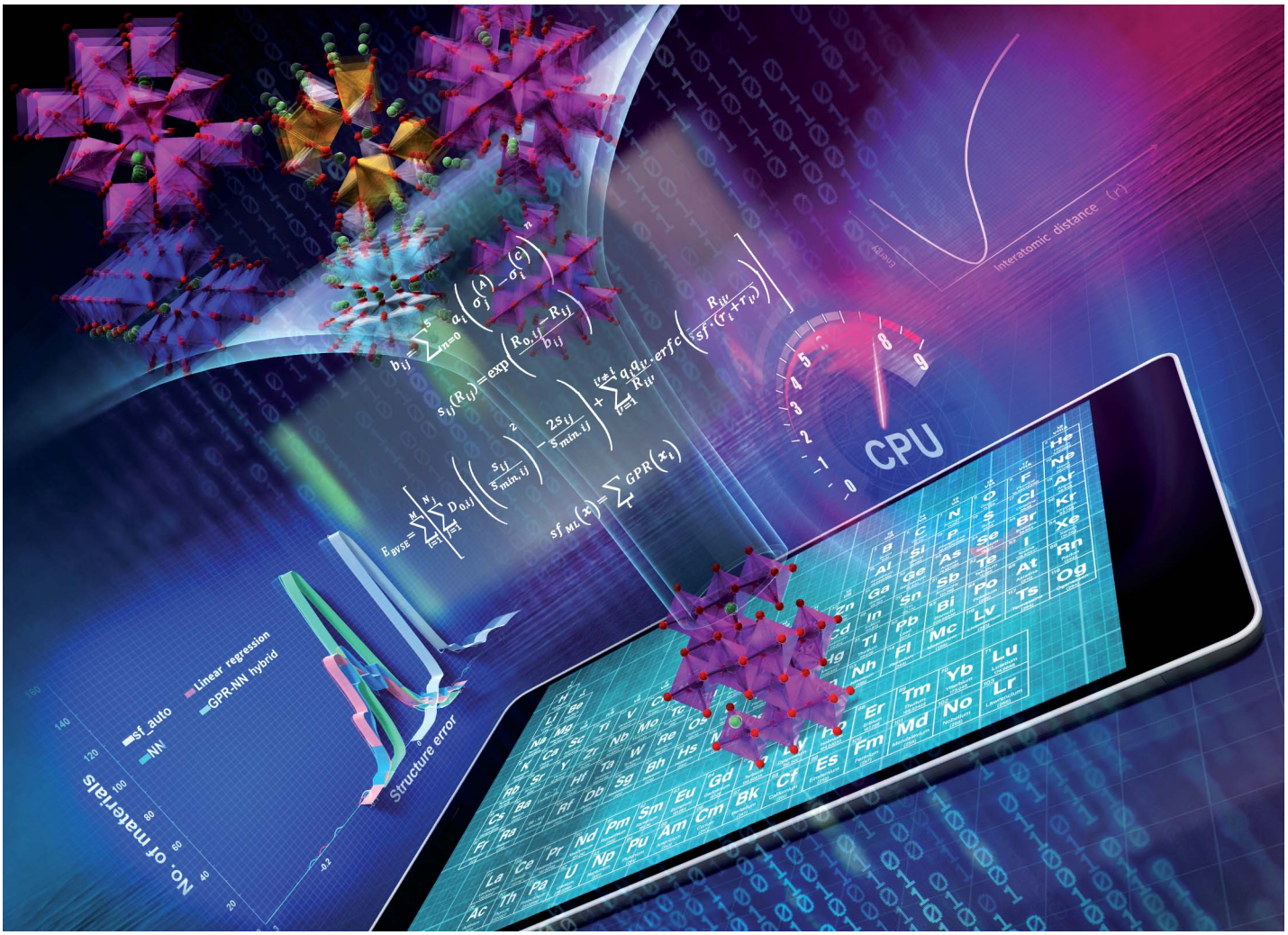

Showcasing research from Ihara-Manzhos laboratory, School of Materials and Chemical Technology, Tokyo Institute of Technology, Tokyo, Japan.

Machine learning the screening factor in the soft bond valence approach for rapid crystal structure estimation

Rapid pre-screening of functional ceramics is needed for multiple applications. The soft bond valence (SoftBV) approach is attractive for this purpose, but its accuracy is limited for both structure and property predictions. We address the issue of structure prediction with SoftBV by machine learning the screening factor – an independent parameter in SoftBV – as function of composition. The recently proposed GPR-NN method, a hybrid between neural network and kernel regression, showed substantial improvement over off-the-shelf ML methods, enabling the prediction of structural parameters with accuracy on the order of 1%.

As featured in:

See Kameda *et al.*, *Digital Discovery*, 2024, **3**, 1967.

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