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From Composition to Crystal: Predicting Sodium-Ion Battery Material Symmetries Using Physics-Guided Machine Learning

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Keletso Monareng1, Petros Ntoahae1, and Rapela Maphanga2,3

1Department of Physics, University of Limpopo, Private bag x 1106, Sovenga, 0727, Polokwane, South Africa
2Next Generation Enterprises and Institutions, Council for Scientific and Industrial Research, P.O. Box 395, Pretoria, 0001, South Africa
3 National Institute for Theoretical and Computational Sciences, NITheCS, Gauteng, 2000, South Africa

Abstract
Sodium-ion batteries (SIBs) have emerged as a promising alternative to lithium-ion systems due to the abundance of Na in Earth's crust and cost-effectiveness. A critical challenge in advancing SIB technology lies in predicting suitable cathode materials and their crystal structures from chemical compositional space. Predicting the crystallographic symmetry of materials from chemical composition remains a central challenge in condensed matter physics and materials science. Traditional methods require detailed structural data, making the discovery process cumbersome. To address this, machine learning (ML) offers a data-driven pathway for rapid and accurate predictions using only elemental information. This study presents a robust, physics-guided ML framework for classifying crystallographic symmetry groups specifically space groups, crystal systems, point groups, and Bravais lattices from chemical formulas of binary and ternary compounds relevant to sodium-ion battery applications. A minimal, physically meaningful feature set was used, including stoichiometry, ionic radii, ionization energies, and oxidation states. The classification task was treated as a multi-label, multi-class problem, and model training addressed data imbalance using weighted metrics. The trained classifiers achieved weighted balanced accuracies exceeding 90% across all symmetry group types. Despite the reduced feature dimensionality, the models consistently captured underlying physical trends, demonstrating high reliability. Comparative analyses revealed that performance scales with dataset size, with ternary compounds yielding higher prediction accuracy than binary ones due to richer data availability. This work underscores the potential of employing physics-informed ML models to accelerate crystal structure prediction directly from chemical formulas, serving as a foundational step toward full geometry prediction and faster discovery of novel materials.

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Primary author: MONARENG, Keletso (University of Limpopo)

Co-authors: Dr NTOAHAE, Petros (University of Limpopo); Prof. MAPHANGA, Regina (Council of Scientific and Industrial Research (CSIR))

Presenter: MONARENG, Keletso (University of Limpopo)

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