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Machine Learning in Inorganic Materials Chemistry

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Message from the Guest Editor

Machine learning (ML) algorithms are increasingly used to solve basic problems in physics and chemistry. In the recent years, ML-based techniques have begun to identify promising synthesis targets from the wide space of candidate compositions. Atomic, molecular, and materials properties have been successfully "machine-learned"; this includes, but is not limited to, atomization energies, band gaps, or NMR chemical shifts. Finally, ML-based interatomic potentials (force fields) are becoming increasingly popular: by fitting to accurate quantum-mechanical reference data, these ML-driven simulation methods can create structural models of materials with an unprecedented combination of accuracy and speed. Today, these methods are beginning to be applicable to questions in solid-state and materials chemistry. It is hoped that this Special Issue will inspire new work at the intersection of ML-driven techniques, solid-state and materials chemistry, and neighboring research fields.

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Message from the Editor-in-Chief

Inorganic chemistry remains a lynchpin of modern chemistry, not only embracing the function and reactivity of combinations of most elements of the periodic table, but also providing a footing for studies of materials, catalysts, drugs, fuels and industrial chemicals. Arguably, the role and reach of inorganics in society have never been as great as today. Adventurous research at the heart and at the extremes of inorganic chemistry is vital to further advances and Inorganics offers authors the opportunity to publish exciting new research in an open access format.

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