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Machine Learning and Materials Informatics

Guest Editors:

Prof. Dr. Yuqing Lin
School of Mechatronical Engineering, Beijing Institute of Technology, Beijing 100081, China

Dr. Shruba Gangopadhyay
Department of Materials Science and Engineering, University of Virginia, Charlottesville, VA 22904-4259, USA

Dr. Aniruddha Dutta
Smith School of Business, Queen's University, Kingston, ON, Canada

Deadline for manuscript submissions:
closed (31 August 2020)

Message from the Guest Editors

Propelled by multiple big data repositories and algorithmic development, machine-learning (ML)- and deep-learning-focused methods are becoming almost indispensable for predicting novel materials and their properties. These methods often rely on the use of already existing datasets to train a computer and map it to new materials or the material property of interest. Earlier prediction endeavors include ML models for the thermodynamic, mechanical and thermal properties of materials. Today high dimensional data from sophisticated atomic-scale resolution instruments are being used to train, test, and predict the shape and important characteristic features of nanomaterials. We are looking forward to compiling a comprehensive set of publications aiming to highlight the latest findings in material science using ML algorithms. We welcome original research involving material discovery, structure–property prediction, material characterization and software development. We invite contributions involving the development, characterization and simulation studies of nanomaterials, biomaterials, and electronic materials along with novel techniques in data preprocessing and feature selection.

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Editor-in-Chief

Prof. Dr. Jamal Jokar Arsanjani
Geoinformatics and Earth Observation Research Group, Department of Planning, Aalborg University Copenhagen, A.C. Meyers Vænge 15, DK-2450 Copenhagen, Denmark

Message from the Editor-in-Chief

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Contact Us

Data Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
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