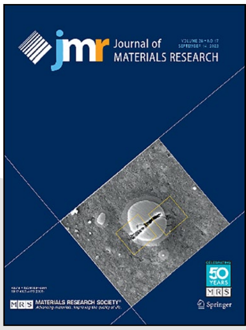


Machine-learned interatomic potentials: Recent developments and prospective applications

Volker Eyert, Jonathan Wormald, William A. Curtin, Erich Wimmer

The authors provide an overview of the state of the art of machine-learned potentials in materials research by presenting a range of impressive applications including metallurgy, photovoltaics, proton transport, nanoparticles for catalysis, ionic conductors for solid-state batteries, and crystal structure predictions. These investigations provide insight into the current challenges and present pathways for their solutions, thus setting the stage for exciting perspectives in computational materials research. https://doi.org/10.1557/s43578-023-01239-8

A machine-learning potential-based generative algorithm for on-lattice crystal structure prediction

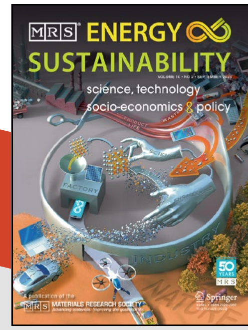
Vadim Sotskov, Evgeny V. Podryabinkin, Alexander V. Shapeev

The authors propose a crystal structure prediction method based on a novel structure generation algorithm and on-lattice machine-learning interatomic potentials. The advantages to this approach include focusing on low-energy structures, reducing computational costs, and significantly reducing the number of density functional theory calculations. Due to the method's computational efficiency, the authors anticipate it paving the way for the efficient high-throughput discovery of multicomponent materials. https://doi.org/10.1557/s43578-023-01167-7

Accelerating training of MLIPs through small-cell training

Jason A. Meziere, Yu Luo, Yi Xia, Laurent Karim Béland, Mark R. Daymond, Gus L.W. Hart

While machine-learned interatomic potentials (MLIPs) have become a mainstay for modeling materials, designing training sets that lead to robust potentials is challenging. Automated methods construct reliable training sets but can be resource-intensive. Current training approaches often use density functional theory calculations that have the same cell size as the simulations that the potential is explicitly trained to model. The authors demonstrate an easy-to-implement small-cell training protocol that decreased training time by approximately 20 times compared to traditional active learning. https://doi.org/10.1557/s43578-023-01194-4



Materials scarcity during the clean energy transition: Myths, challenges, and opportunities

Anthony Y. Ku, Elizabeth A. Kocs, Yoshiko Fujita, Andrew Z. Haddad, Robert W. Gray IV

Open Access

The MRS Focus on Sustainability Subcommittee sponsored a panel discussion on innovation in materials science and engineering to support supply chains for clean energy technologies. The authors examine the myth of materials scarcity, explain the need for innovation in materials in helping supply chains dynamically adapt over time, and show how the materials research community can effectively engage with industry, policymakers, and funding agencies to drive the needed innovation in critical areas. https://doi.org/10.1557/s43581-023-00077-9

A critical review of current conversion facilities and research output on carbon dioxide utilization

Victor Joseph Aimikhe, Majid Abiodun Adeyemi

The authors present a literature survey on global CO_2 utilization facilities based on location and product type, and recent publications on CO_2 conversion to value-added products. They conclude that most CO_2 conversion facilities produce chemical intermediates, polymers, urea, and building materials, while most research output focuses on CO_2 conversion to chemical intermediates, polymers, building materials, and fuels. They present the need to increase CO_2 conversion facilities and research output on fuel synthesis to aid decarbonization efforts. https://doi.org/10.1557/s43581-023-00073-z

Carbon footprint inventory using life cycle energy analysis

Ching-Feng Chen, S.K. Chen

The authors conduct a carbon footprint inventory (CFI) case study of the most extensive 181-MWp offshore floating photovoltaic deployment at Taiwan's Changhua Coastal Industrial Park station using a high-quality management system. The results show the project will produce 4529.2 GWh over 25 years and subside approximately 2305.4 kilo-tons (kt) of CO_2 emission. The findings help photovoltaic systems' CFI and decision-makers determine energy infrastructure strategies. https://doi.org/10.1557/s43581-023-00074-y

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