

MaterialsAtlas.org: a materials informatics web app platform for materials discovery and survey of state-of-the-art

Jianjun Hu, Stanislav Stefanov, Yuqi Song, Sadman Sadeed Omee, Steph-Yves Louis, Edirisuriya M. D. Siriwardane, Yong Zhao & Lai Wei

<https://doi.org/10.1038/s41524-022-00750-6>

Abstract

The availability and easy access of large-scale experimental and computational materials data have enabled the emergence of accelerated development of algorithms and models for materials property prediction, structure prediction, and generative design of materials. However, the lack of user-friendly materials informatics web servers has severely constrained the wide adoption of such tools in the daily practice of materials screening, tinkering, and design space exploration by materials scientists. Herein we first survey current materials informatics web apps and then propose and develop MaterialsAtlas.org, a web-based materials informatics toolbox for materials discovery, which includes a variety of routinely needed tools for exploratory materials discovery, including material's composition and structure validity check (e.g. charge neutrality, electronegativity balance, dynamic stability, Pauling rules), materials property prediction (e.g. band gap, elastic moduli, hardness, and thermal conductivity), search for hypothetical materials, and utility tools. These user-friendly tools can be freely accessed at <http://www.materialsatlas.org>. We argue that such materials informatics apps should be widely developed by the community to speed up materials discovery processes.