

Materials discovery with artificial intelligence

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Abstract: We have developed a computational tool that employs deep learning to discover new materials. The tool combines Density Functional Theory calculations with experimental results into a holistic materials design tool. The tool has proposed four alloys for use in jet engines, whose properties have been experimentally verified, a Lithium-ion battery cathode, and been used to probe the integrity of a commercial materials database.

More info: http://www2.warwick.ac.uk/fac/sci/wcpm/seminars



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